

## GROMACS - Bug #298

### Segfault in a parallel particle decomposition run

02/22/2009 12:51 PM - Ondrej Marsalek

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Erik Lindahl	
<b>Category:</b> mdrun	
<b>Target version:</b> 4.0	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	
<b>Description</b>	
Created an attachment (id=354) tpr file that produces the error	
I have encountered a segmentation fault with Gromacs 4.0.3. It only happens in a parallel run (particle decomposition, open boundary conditions), the same setup runs fine in serial. It also runs fine if I switch the thermostat to Berendsen instead of v-rescale.	
The command that produces the error was: mpirun -np 2 mdrun_d -pd -s w.tpr	
I use OpenMPI 1.3 and the Intel compiler on a Core2 machine. I can provide more information if needed.	
I attach the tpr file.	
The stack trace was:	
starting mdrun 'Neat water' 500000 steps, 500.0 ps. [isis:23154] * <b>Process received signal</b> [isis:23154] Signal: Segmentation fault (11) [isis:23154] Signal code: Address not mapped (1) [isis:23154] Failing at address: (nil) [isis:23154] [ 0] /lib/libpthread.so.0 [0x7f41e64050f0] [isis:23154] [ 1] /opt/gromacs-4.0.3/double/lib/libmd_mpi_d.so.5(vrescale_tcoupl+0x184) [0x7f41e8b3048c] [isis:23154] [ 2] /opt/gromacs-4.0.3/double/lib/libmd_mpi_d.so.5(update+0x1fa) [0x7f41e8bad03c] [isis:23154] [ 3] mdrun_d(do_md+0x25f9) [0x416ed1] [isis:23154] [ 4] mdrun_d(mdrunner+0xf35) [0x419bd3] [isis:23154] [ 5] mdrun_d(main+0x55f) [0x41a35f] [isis:23154] [ 6] /lib/libc.so.6(__libc_start_main+0xe6) [0x7f41e60a2466] [isis:23154] [ 7] mdrun_d [0x4062d9] [isis:23154] <b>End of error message</b> *	
----- mpirun noticed that process rank 1 with PID 23154 on node isis exited on signal 11 (Segmentation fault). -----	

#### History

##### #1 - 02/25/2009 04:19 PM - Berk Hess

This bug is not directly related to particle decomposition.  
The thermostat integral flag for the state was not set with pbc=none.  
This causes a segv with particle decomposition.  
I fixed it.  
The fix is below if you need it.

Berk

RCS file: /home/gmx/cvs/gmx/src/mdlib/init.c,v

retrieving revision 1.59.2.1

diff r1.59.2.1 init.c

125,127c125,127

< if (ir->etc etcNOSEHOOVER || ir->etc etcVRESCALE) {

< state->flags |= (1<<estTC\_INT);

< }

-

}

if (ir->etc etcNOSEHOOVER || ir->etc etcVRESCALE) {  
state->flags |= (1<<estTC\_INT);

## Files

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w.tpr	7.55 KB	02/22/2009	Ondrej Marsalek
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