GROMACS - Bug #85

mdrun with PME gives different results with MPI

06/01/2006 08:20 PM - David van der Spoel

Status:	Closed			
Priority:	High			
Assignee:	David van der Spoel			
Category:	mdrun			
Target version:	3.3.1			
Affected version - extra info:		**Difficulty:**	uncategorized	
Affected version:				

Description

When mdrun is run from mpirun as
mpirun -c 1 mdrun -s
it gives different results than when run as
mdrun -s
and when it is compiled without MPI it gives yet different results.
The differences are very minor and are due to PME. Currently we suspect that it
has to do with bsplines stuff

History

#1 - 07/12/2006 03:52 PM - Anonymous

Compiling with: ./configure --with-fft=fftpack(or fftw3) --without-x
and compiling with an additional line of #define DEBUG in src/mdlib/pme.c also
gives different results. Maybe it is caused by the same bug.

The difference is also very small. Running mdrun -debug resulted in different
adresses for Grid and different entries at some locations in the qgrid array.

I checked that the adress does not change after the memory allocation.

After this I suspected that somewhere a pointer array is exceeded (because
adding fprintf statements in pme.c could result in changing the manifestation of
the bug) and the information is put into the Grid memory area. So I compiled
with dmalloc, but it did not give any out of bounds warnings.

However dmalloc does not check for static pointer arrays. Maybe the problem is
in one of the static pointer arrays, but I do not know how to check them.

Same problem can occur when implementing new force functions.

#2 - 09/11/2007 12:07 PM - David van der Spoel

I can not reproduce this bug anymore, neither with the 3.3 CVS or the 4.0 CVS code. (Not with vanilla 3.2.1 either). This could have been caused by
compilation issues. Tested on both Mac an Linux box.