GROMACS - Bug #9

mdrun exits on reading tpr files for >1 CPU on linux pc

09/06/2005 01:55 PM - Carsten Kutzner

Status:	Closed		
Priority:	High		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	3.3_rc1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Successfully installed Gromacs 3.3rc1 on 2.4.21 linux. Single processor tpr files run as expected. When running mdrun in parallel, it always crashes with errors like:

```
Reading file ../TEST.tpr, VERSION 3.3_rc1 (single precision)
------------------------------------------------------------
Program mdruncvs, VERSION 3.3_rc1
Source code file: block_tx.c, line: 74

Fatal error:
0: size=4, len=12, rx_count=0

------------------------------------------------------------
```

(Size and len vary depending on tpr file used)

```
Reading file ../AP-100steps-04s.tpr, VERSION 3.2.90_beta_20040828 (single precision)
------------------------------------------------------------
Program mdrun, VERSION 3.3_rc1
Source code file: symtab.c, line: 108

Fatal error:
symtab get_symtab_handle 81527 not found
------------------------------------------------------------
```

- gmx configure flags --enable-mpi --without-x --disable-x
- LAM 7.1.1
- AMD Athlon dual proc
- gcc version 3.3.1, gnu c lib 2.3.3
- tried both the cvs version and the gmx 3.3rc1 tar file
- tested 3 different systems / input tpr files

History

#1 - 09/06/2005 02:00 PM - Carsten Kutzner

Created an attachment (id=1)
tpr file of guanylin test system for 2 CPUs

try something like
mpirun -np 2 ~/gromacs-3.3_rc1/src/kernel/mdrun -s ../guanylin-02.tpr

#2 - 09/06/2005 03:36 PM - Erik Lindahl

This is caused by an error in the QM-MM group communication. Will fix!

#3 - 09/06/2005 03:57 PM - Erik Lindahl

The QM group data were send after the annealing data, but received before.

Files