GROMACS - Bug #1313

g_tune_pme hangs when using new IBM PE

07/31/2013 06:33 PM - Carsten Kutzner

| Status:     | Closed            |
| Priority:   | Normal            |
| Assignee:   | Carsten Kutzner  |
| Category:   | mdrun             |
| Target version: | 4.6.4         |
| Affected version - extra info: | |
| Affected version: | 4.6              |
| Difficulty: | uncategorized     |

Description
If one uses g_tune_pme with the new version of IBM MPI, runs on larger number of nodes (>= 8) in most cases never do any tuning but hang.
The hang happens when g_tune_pme checks with a system call whether it can execute mdrun, and therefore calls mdrun -h.
Even a simple c program making a system call with "poe mdrun -h" produces these hangs on IBM PE.

IBM PE does not seem to like the exit(0) after gmx_print_version_info() in statutil.c. If one however properly shuts down the MPI universe by adding a gmx_finalize_par() just before the exit(0), IBM PE is happy. I guess there should not be any side effects by adding a gmx_finalize_par() there, since the gmx_finalize_par() only calls MPI_Finalize if MPI_Initilized() returns true.

Associated revisions
Revision 68d75a4a - 08/01/2013 08:46 AM - Carsten Kutzner
Properly finalize MPI on mdrun -version. Fixes #1313
Change-Id: l1ae5f342da96980df322770d134555e2dc9fe712

History
#1 - 07/31/2013 07:30 PM - Carsten Kutzner
Sorry, I meant "mdrun -version" instead of "mdrun -h".

#2 - 08/01/2013 11:22 AM - Carsten Kutzner
- Status changed from New to Resolved

#3 - 08/01/2013 11:22 AM - Carsten Kutzner
- Status changed from Resolved to Closed