GROMACS - Bug #1313

%tune_pme hangs when using new IBM PE

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

<table>
<thead>
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<th>Closed</th>
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<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Carsten Kutzner</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.4</td>
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<td>Affected version - extra info:</td>
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**Description**

If one uses %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_Initialed() returns true.

**Associated revisions**

Revision 68d75a4a - 08/01/2013 08:46 AM - Carsten Kutzner

Properly finalize MPI on mdrun -version. Fixes #1313

Change-Id: I1ae5f342da96980df322770d134555e2dc9fe712

**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