Gromacs - Bug #1319

**g_tune_pme assumes an MPI environment is available**

08/09/2013 05:35 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.4</td>
</tr>
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<td>Affected version</td>
<td>4.6.3</td>
</tr>
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<td>extra info:</td>
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**Description**

`g_tune_pme -np 512 -nobench` fails on machines (like BlueGene/Q) where you can only get an MPI environment via the queueing system. The routine that checks that mdrun works assumes it can do that check by running a quick MPI program, and does so regardless of `-nobench`.

**Associated revisions**

Revision b8c79db2 - 09/19/2013 10:27 AM - Mark Abraham

Fixed `g_tune_pme` assumption that MPI is available

Refactored function with two distinct parts into two functions. This makes it easy to call the part that checks that mdrun works only when that check is necessary. Now `g_tune_pme -np 512 -nobench` works on machines like BlueGene/Q where you might only be able to get the MPI environment via the queueing system. `g_tune_pme -nobench` should work as a stand-alone.

Fixes #1319

Change-Id: I7237800a1c67664c9253e5422a7b3f12f4ebd62f

**History**

#1 - 08/09/2013 05:57 PM - Mark Abraham

- Status changed from In Progress to Fix uploaded

#2 - 09/19/2013 10:30 AM - Mark Abraham

- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset b8c79db25cc22892257b917ce1f0b10d57e68ac6.

#3 - 10/16/2013 01:49 PM - Mark Abraham

- Status changed from Resolved to Closed