GROMACS - Bug #1319

g_tune_pme assumes an MPI environment is available
08/09/2013 05:35 PM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: mdrun
Target version: 4.6.4
Affected version - extra info: all to date
Affected version: 4.6.3

Difficulty: uncategorized

Description

g_tune_pme -np 512 -nobench fails on machines (like BlueGene/Q) where you can only get an MPI environment via the queuing 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 queuing 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 b8c79db25cc22892257b917ce1f6b10d57e68ac6.

#3 - 10/16/2013 01:49 PM - Mark Abraham
- Status changed from Resolved to Closed