Incorrect warning about PME ranks during cpt restart

11/30/2017 11:26 PM - Erik Lindahl

Status: Closed
Priority: Normal
Assignee: mdrun
Category: mdrun
Target version: 2018
Affected version - extra info:
Affected version: 2018
Difficulty: simple

Description
When restarting from a checkpoint and using the same setup with separate PME ranks as for the checkpoint, gromacs incorrectly warns about PME rank mismatching, and thinks the current run does not use separate PME ranks.

History
#1 - 12/08/2017 03:20 PM - Paul Bauer
Hello, I have been trying to reproduce this using a small test system and the beta release version, but no luck. Could you send me the way you set up the simulation?
Thanks!

#2 - 12/10/2017 06:25 PM - Erik Lindahl
It might have been fixed by Mark's other patch for selecting PME nodes automatically. Will test tonight.

#3 - 12/11/2017 09:16 AM - Berk Hess
I think I noticed this issue as well around the time this got filed. But now I can not reproduce it with the code from around that time and neither with current HEAD of release-2018.

#4 - 12/11/2017 10:10 AM - Mark Abraham
I assume this is fixed, but haven't tried

#5 - 12/11/2017 12:09 PM - Erik Lindahl
- Status changed from New to Resolved

Fixed by Mark's change to fix the separate PME node assignment.

#6 - 12/11/2017 12:09 PM - Erik Lindahl
- Status changed from Resolved to Closed