Gromacs - Bug #1169
PME load balancing cut-off issues
02/28/2013 06:08 PM - Berk Hess

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 4.6.1
Affected version - extra info: 4.6

Description
At the initial stage of the PME load balancing the domain decomposition dynamic load balancing can make cells smaller than the cut-off. This could potentially lead to missing interaction during a very limited number of steps. But this bug mainly reduces the effectiveness of the PME load balancing

Associated revisions
Revision e348e56a - 03/05/2013 08:19 PM - Berk Hess
fixed bug with DD cut-off check and PME DLB

During the initial stage of PME DLB, the cut-off limit check for the DD DLB was not checked correctly. This reduced the effectiveness of both DD and PME DLB and could lead to missing interactions during a very limited number of steps.
Fixes #1169
Change-Id: I0b0cac22d4abbe8a9b0c16488aeb662d7d4d9bcc

Revision 31725cfc - 06/13/2013 09:45 AM - Berk Hess
fixed bug with DD cut-off check and PME DLB

During the initial stage of PME DLB, the cut-off limit check for the DD DLB was not checked correctly. This reduced the effectiveness of both DD and PME DLB and could lead to missing interactions during a very limited number of steps.
Fixes #1169
Change-Id: I0b0cac22d4abbe8a9b0c16488aeb662d7d4d9bcc

History
#1 - 03/06/2013 02:40 PM - Berk Hess
- Status changed from New to Closed