Gromacs - Bug #1416

2-D Ewald summation and DD is broken

01/05/2014 12:29 AM - Justin Lemkul

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: future

Affected version: 4.5.5

Description

Energy drift reported on gmx-users:


Reported in version 4.5.5, may affect more recent versions. Apparently it is a problem in DD, as running with PD resolves the issue:


With PD slated for removal, I figured it was important to note it here. Related to issue #1292.

Related issues:
Related to Gromacs - Feature #1292: mdrun features to deprecate for 5.0

History

#1 - 01/05/2014 12:29 AM - Justin Lemkul
- Related to Feature #1292: mdrun features to deprecate for 5.0 added

#2 - 06/23/2015 03:38 PM - Berk Hess
- Status changed from New to Closed

There are issues when molecules are broken over PBC in Z. If you only have molecules with net charge zero, PD will give correct results. But the general issue can not be solved, since with charged molecules the dipole of the system can not be uniquely defined. So we will not solve this. In newer versions grompp will warn you about this.

If you think there is caused by something else, please reopen the issue.