GROMACS - Bug #3441

Ewald surface-epsilon is incorrect

03/11/2020 05:04 PM - Berk Hess

Status: Resolved
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2020.2
Affected version - extra info:
Affected version: 2020.1

Difficulty: uncategorized

Description
The Ewald surface-epsilon correction term is incorrect when molecules are broken over PBC. It should be disabled in the 2020 release.

Associated revisions

Revision c4878aff - 03/17/2020 08:47 AM - Berk Hess
Disable Ewald dipole correction without DD

Refs #3441

Change-id: l492cd136b41e57b3e2198c110717177f4d46a7c

Revision 2548c9e0 - 03/18/2020 11:04 PM - Berk Hess
Use WholeMoleculeTransform for orires and epsilon-surface

Remove direct use of the graph from the orientation restraint and Ewald epsilon-surface term code by passing in whole molecules created by the WholeMolecules class. Since this was the only remaining use of graph in do_force(), it can now be removed.

Also enabled the epsilon-surface mdrun-test.

Fixes #3441

Change-id: ldfe65086d6d9e1a656cf23613ede3793794901

History

#1 - 03/18/2020 11:15 PM - Berk Hess
- Status changed from Accepted to Resolved

Applied in changeset 2548c9e0e0ce93d295e10d95310763f7700ea7d17.