update cut-off treatment checks and documentation, especially PME-switch

03/07/2013 12:01 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: preprocessing (pdb2gmx,grompp)
Target version: 4.6.3
Affected version - extra info: 4.6.1
Affected version: 4.6.1

Description

grompp still advises to use PME-switch when running NVE simulations. But PME-switch is deprecated, as we now have exact cut-off's with the Verlet scheme and they can also be used with the group scheme. The confusing effect of the potential-modifier on the cut-off behavior with the group scheme is not reflected in the grompp warnings and mdp-opt.html.

Associated revisions

Revision f780dc8 - 05/21/2013 06:40 PM - Mark Abraham
Updated grompp cut-off and PME-Switch checks
Added a warning with PME-Switch when switching over more than 5%. Charge-group size rlist notes/warnings now also appear when potential modifiers are used. Documented effect of potential-modifiers on the group scheme cut-off treatment in mdp_opt.html.

Fixes #1179
Change-Id: lde00caf5ae378104f99611bf197e896d1b53d7d7

Revision c1e94319 - 06/13/2013 09:45 AM - Mark Abraham
Updated grompp cut-off and PME-Switch checks
Added a warning with PME-Switch when switching over more than 5%. Charge-group size rlist notes/warnings now also appear when potential modifiers are used. Documented effect of potential-modifiers on the group scheme cut-off treatment in mdp_opt.html.

Fixes #1179
Change-Id: lde00caf5ae378104f99611bf197e896d1b53d7d7

History

#1 - 04/30/2013 05:10 PM - Mark Abraham
- Status changed from In Progress to Fix uploaded
- Affected version set to 4.6.1

#2 - 04/30/2013 06:13 PM - Michael Shirts
I'm still suspicious about exact cutoffs for free energy calculations, but it's on me to show that there's an issue. One of the list of things that needs to be done in the next week or two.

#3 - 05/21/2013 06:45 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 7780dc633f55d588f0fbc049af667519d9cf868e.
#4 - 05/21/2013 06:50 PM - Mark Abraham
- Status changed from Resolved to In Progress

Ongoing debate about this issue in https://gerrit.gromacs.org/2220

#5 - 05/22/2013 05:07 AM - Mark Abraham
- Target version changed from 4.6.2 to 4.6.3

#6 - 06/13/2013 09:55 AM - Mark Abraham
- Status changed from In Progress to Resolved

Applied in changeset c1e94319d4cf2ad5318abf3c63a0dad994e5624a.

#7 - 12/16/2013 05:40 PM - Rossen Apostolov
- Status changed from Resolved to Closed