GROMACS - Feature #1231

single-point energies

04/25/2013 12:56 PM - Mark Abraham

Status: Closed
Priority: Low
Assignee: Erik Lindahl
Category: preprocessing (pdb2gmx,grompp)
Target version: 5.0
Difficulty: uncategorized

Description
New users always seem to assume a zero-step MD is a single-point energy, but this is only true with unconstrained-start having the right value.
grompp should warn when the erroneous combination is used.
grompp should note in either case that mdrun -rerun should be used.
IIRC zero-step EM already does some similar output. Not sure whether that is in mdrun or not - if so, move to grompp.

Associated revisions
Revision f3c4bd6b - 06/23/2014 10:47 AM - Erik Lindahl
 Warn if using nsteps=0 without continuation=yes

To achieve true single-point energy evaluations for a structure we should not constrain the initial conformation. This is typically done by settings nsteps=0, so grompp now warns if this is used while keeping continuation = no (the default).

Fixes #1231.

Change-Id: I4e65b66f6535da4206e7dbd5f7769a33c94ec12d

History
#1 - 05/01/2013 01:22 AM - Mark Abraham
Also treat mdrun -nstep 0 the same way as .mdp setting nsteps = 0

#2 - 06/26/2013 01:32 AM - Mark Abraham
- Target version set to 4.6.4

#3 - 10/16/2013 01:46 PM - Mark Abraham
- Target version changed from 4.6.4 to 4.6.x

#4 - 06/12/2014 01:21 AM - Erik Lindahl
- Tracker changed from Bug to Feature

#5 - 06/18/2014 02:25 PM - Mark Abraham
- Target version changed from 4.6.x to 5.x

#6 - 06/23/2014 12:04 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1231.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I4e65b66f6535da4206e7dbd5f7769a33c94ec12d
Gerrit URL: https://gerrit.gromacs.org/3655

#7 - 06/23/2014 02:16 PM - Erik Lindahl
- Status changed from New to Resolved
#8 - 06/23/2014 02:16 PM - Erik Lindahl
  - Status changed from Resolved to Closed

#9 - 07/15/2014 06:44 AM - Teemu Murtola
  - Assignee changed from Mark Abraham to Erik Lindahl
  - Target version changed from 5.x to 5.0