Gromacs - Bug #1208

Genion should treat a combination of -nn (or -np) with -conc better

03/24/2013 06:20 PM - Mark Abraham

Status: Closed
Priority: Low
Assignee:
Category: preprocessing (pdb2gmx,grompp)
Target version: 4.6.3

Description
Documentation for genion -conc notes that it overrides -nn and -np, but the output should say something specific about what is happening.


Associated revisions
Revision 9b57187d - 06/06/2013 08:24 PM - Pedro Lacerda
Various fixes for genion
Remove genion non-random insertion of ions, by side effect it stops writing useless log file. This commit also warns user about -conc option overriding -nn or -np.
Fixes #1236, #615, and #1208
Change-Id: lcb7e411cda10abb3a77ea4137534f253b0777def

History
#1 - 05/22/2013 05:42 AM - Mark Abraham
- Status changed from New to Fix uploaded
- Assignee changed from Berk Hess to Mark Abraham
- Target version changed from future to 4.6.2
- Affected version set to 4.6.1

Fixed in commit e86aa93597dcacbb2e25ace177dc8daf24c7f4f0c. Thanks Pedro Lacerda!

#2 - 05/22/2013 05:42 AM - Mark Abraham
- Status changed from Fix uploaded to Resolved

#3 - 05/22/2013 08:04 PM - Teemu Murtola
- Status changed from Resolved to Feedback wanted

I don't think that the mentioned commit actually addresses the problem reported here: it affects how -neutral interacts with the various options, but does not alter the output in the reported case in any way.

From the code, it seems that genion already prints out the number of ions it intends to add (and that may be different from those given with -nn and/or...
-np), but perhaps it should be even more explicit.

#4 - 05/31/2013 10:44 AM - Mark Abraham
- Assignee deleted (Mark Abraham)
- Target version changed from 4.6.2 to 4.6.x

#5 - 06/07/2013 06:50 AM - Pedro Lacerda
I added an warning about -conc overriding -nn or -np in the associated revision. I'm happy you accepted my changes.

I thought that the commit line "Fixes ..." would close this issue automatically. It was because "and" preceded the issue ID, or because the status is "feedback wanted"?

#6 - 06/07/2013 03:20 PM - Mark Abraham
- Status changed from Feedback wanted to Resolved

Probably the "and." We are working on a fancier mechanism here.

#7 - 07/05/2013 06:33 PM - Mark Abraham
- Status changed from Resolved to Closed

#8 - 07/05/2013 06:35 PM - Mark Abraham
- Target version changed from 4.6.x to 4.6.3