

GROMACS - Feature #1236

deprecate genion non-random insertion of ions

05/01/2013 12:46 AM - Mark Abraham

Status:	Closed	
Priority:	Low	
Assignee:	Mark Abraham	
Category:	preprocessing (pdb2gmx,grompp)	
Target version:	4.6.3	
Difficulty:	uncategorized	
Description		
This feature has been announced as buggy since at least 2006. I'm struggling to see much use for it anyway. Its code surely does not work any more.		
Related issues:		
Related to GROMACS - Bug #615: genion writes a log file	Closed	11/20/2010

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: Icb7e411cda10abb3a7fea4137534f253b0777def

History

#1 - 06/06/2013 08:25 PM - Pedro Lacerda

- Status changed from *New* to *Resolved*
- % Done changed from 0 to 100

Applied in changeset [9b57187d48cd10e27e818ef32567b6f9be74d506](#).

#2 - 06/26/2013 01:49 PM - Mark Abraham

- Target version changed from 5.0 to 4.6.3

#3 - 12/16/2013 05:40 PM - Rossen Apostolov

- Status changed from *Resolved* to *Closed*