

GROMACS - Task #1373

Add missing nbxn tests

10/30/2013 04:18 AM - Roland Schulz

Status:	New
Priority:	Low
Assignee:	Mark Abraham
Category:	testing
Target version:	
Difficulty:	uncategorized
Description	
We probably don't want/need to test all kernels, but we probably want to test each kernel option (e.g. ewald/ff/tab, geom/lb/none) once. comb_none isn't tested. Others might be missing too.	

History

#1 - 10/30/2013 09:23 AM - Mark Abraham

Ja, I have had some stuff suitable for unit-style tests for these kinds of combinations for a few months. Will try to get them working again this week, now that the release-4-6 stuff has made its way up.

#2 - 10/31/2013 11:27 PM - Mark Abraham

Some stuff uploaded in <https://gerrit.gromacs.org/#/c/2489/>, but would need to be expanded to treat all the kernels.

#3 - 06/09/2014 08:36 PM - Erik Lindahl

- *Priority changed from Normal to Low*

It might be worth considering bug 1370 here. While it appeared completely safe to add a CMake option to auto-download all regression tests this is now causing problems for Gentoo, due to timeouts on ARM.

For now, I would strong vote NOT to add more unit tests that are complete MD simulation, primarily because they simply aren't unit tests. If things are to go in the unit tests, they should only test a single force evaluation to make sure the functional form is correct.