Shell code in single precision gives non-reproducible forces

For the complex/sw test adding reference values for the forces causes it to be non-reproducible between different build configurations. See https://gerrit.gromacs.org/#/c/1259/ for details. It should be checked whether that is caused by some bug in the code or whether it is expected. If it is expected the test should be adapted. For now the test doesn't have reference values for single precision forces (and thus the forces aren't tested).

Associated revisions

Revision f1b89b02 - 08/10/2012 05:03 AM - Roland Schulz
Check forces for all tests
Forces wasn't written out for most tests and thus not tested.
Reference values are generated with 4.5.5
The complex/sw/reference_s.trr still does not contain forces because of #993.
Change-Id: I8908ea9d97ae5b0ef018d13aee99bf09f5087bfd

History

#1 - 09/14/2012 05:34 PM - Szilárd Páll
- Category set to mdrun
- Target version set to 4.6

#2 - 10/19/2012 04:43 AM - Roland Schulz
- Status changed from New to Closed

As David explains in 1259 it is most likely a change in order. We should have better tests to also be able to test single precision but that doesn't require its own redmine issue.