### Description

The following expression in "gromacs/gmxlib/nonbonded/nb_generic.cpp":

\[
\text{rinvcorr} = (\text{fr->coulomb}\_\text{modifier} == \text{eintmodPOTSHIFT}) \ ? \ rinv-\text{fr->ic->sh\_ewald} : rinv;
\]

Unit of "rinv" is inverse of nanometer; 
"sh\_ewald" is just a number without unit in that

\[
\text{ic->sh\_ewald} = \text{gmx}\_\text{erfc}((\text{ic->ewaldcoeff}\_q*\text{ic->rcoulomb});
\]

is defined in
"gromacs/mdlib/forcerec.cpp"
or
"gromacs/ewald/pme-load-balancing.cpp"

### Associated revisions

**Revision 3f970c00 - 08/15/2017 01:27 PM - Mark Abraham**

Fix value of Ewald shift

In all the short-ranged kernel flavours, sh\_ewald is subtracted from rinv, which have inconsistent dimensions. Fortunately, rcutoff is often close to 1, and the inconsistent shifts often cancel in practice, and energy differences computed on neighbour lists of the same size will have the error cancel. The difference doesn't even show up in the regressiontests, but would if we had a unit test of a single interaction.

Fixes #2215
Change-Id: Ia2ea57f3bd9d521879783b207353d9d6f4ccb4a8

### History

**#1 - 07/16/2017 03:14 AM - Mark Abraham**

There seems to be a minor, but embarrassing, issue here. sh\_ewald is used as if it was computed as \text{erfc}(\beta \ast \text{cutoff})/ \text{cutoff} but computed only as \text{erf}(\beta \ast \text{cutoff}). Fortunately, cutoff is approximately one, and the errors from opposite charges approximately cancel, and for a given cutoff energy differences will have even more fortuitous cancelling.

I think we should subtract the cutoff distance from sh\_ewald in forcercel.cpp. And plan to use a name that is more descriptive of the quantity, ie that it is a potential shift (albeit in 1/r form).

This issue was introduced along with the Verlet scheme, and now affects the group scheme also, in every Ewald kernel that I have seen.

**#2 - 07/20/2017 09:19 AM - Gerrit Code Review Bot**

Gerrit received a related patchset ‘1’ for Issue #2215.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-5-1~Ia2ea57f3bd9d521879783b207353d9d6f4ccb4a8
Gerrit URL: https://gerrit.gromacs.org/6798

**#3 - 07/31/2017 09:41 PM - Mark Abraham**

- Target version set to 5.1.5
- Affected version changed from 2016.3 to 5.1.5

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02/23/2020
#4 - 08/08/2017 08:27 PM - Berk Hess
- Category set to documentation
- Status changed from New to Fix uploaded

Note that this bug only affects the reported energies, not the forces or the sampling. And, as Mark noted, the effects on the energy are very small, so this is relatively harmless (but still embarrassing).

#5 - 08/15/2017 04:35 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

Applied in changeset 3f970c00ffaf60b47c14003e72f941b429d275b.

#6 - 09/12/2017 11:58 AM - Mark Abraham
- Status changed from Resolved to Closed