potential-shift and previous switch functions combination is either incompatible or bugged

06/06/2013 05:18 AM - Michael Shirts

Description

Probably not that important, since not many people will intentionally do this, but should either be fixed, or people prevented from doing it.

If you try combinations of old switch function style plus potential-shift, the results are very bad for coulomb short range:

Examples:

```
  rlist           = 1.1
  coulombtype     = PME-switch
  rcoulomb-switch = 0.88
  rcoulomb        = 0.90
  vdw-type        = cutoff
  rvdw            = 0.9
  vdw-modifier    = potential-shift
```

Then the first step gives:

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>7804.528862</td>
<td>-486.152949</td>
<td>195147.899480</td>
<td>-5284.241647</td>
</tr>
</tbody>
</table>

Where the coul short range should be -44K.

Now shifted coul, switch vdw

```
  rlist           = 1.1
  coulombtype     = PME
  rcoulomb        = 0.90
  coulomb-modifier = potential-shift
  vdw-type        = switch
  rvdw-switch     = 0.85
  rvdw            = 0.9
```

```
  --------|---------------|--------------|--------------|
  7583.587202 | -264.829383 | 195099.861796 | -5284.241647 |
```

Also bad. For comparison, with BOTH switches, we get:

```
  --------|---------------|--------------|--------------|
  7583.587202 | -426.829383 | -44261.809417 | -5284.241647 |
```

With both potential shift, we get:

```
  --------|---------------|--------------|--------------|
  7804.528862 | -486.152949 | -44261.851488 | -5284.241647 |
```

Big difference!

Either these methods or incompatible and the combination should be disallowed, or the issue identified and fixed.
History

#1 - 10/16/2013 01:46 PM - Mark Abraham
- Target version changed from 4.6.4 to 4.6.x

#2 - 05/22/2014 04:28 PM - Erik Lindahl
- Status changed from New to Closed

Fixed by https://gerrit.gromacs.org/#/c/3477/ and https://gerrit.gromacs.org/#/c/3279/. We're tracking this through redmine #1463 instead.

Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>topol.top</td>
<td>1.7 KB</td>
<td>06/06/2013</td>
<td>Michael Shirts</td>
</tr>
<tr>
<td>confout.gro</td>
<td>209 KB</td>
<td>06/06/2013</td>
<td>Michael Shirts</td>
</tr>
<tr>
<td>grompp.mdp</td>
<td>2.65 KB</td>
<td>06/06/2013</td>
<td>Michael Shirts</td>
</tr>
</tbody>
</table>