GROMACS - Feature #1176

Request for pdb2gmx -water tips3p

03/05/2013 08:37 PM - Chris Neale

<table>
<thead>
<tr>
<th>Status:</th>
<th>Rejected</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
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<td>Target version:</td>
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<td>Difficulty:</td>
<td>uncategorized</td>
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Description

In v4.6, it is not possible to use the -water option to pdb2gmx to get the charmm tip3p water when using the charmm ff (I didn't check the CVS).

It's easy enough to get around this on the command line, but when scripting it is dangerous to do something like:

```
echo 3 | pdb2gmx -f my.gro -ff charmm27
```

because if option 3 changes, one might not notice in an older script.

History

#1 - 03/06/2013 09:27 AM - Berk Hess
- Status changed from New to Feedback wanted

I purposely did not add a tips3p option to pdb2gmx to not encourage the use of this model. It runs twice as slow with the group scheme, and tips3p has even less structure than tip3p, which is already under-structured. We would rather not encourage the use of a bad water model that is also very slow. It is not completely clear to me why Charmm added LJ to the hydrogens. I had heard something about the code not being able to handle particles without LJ, but I don't know if that is true.

So I would like to keep things as they are. If users really want tips3p, they can change a single character in the top file.

#2 - 03/06/2013 03:56 PM - Chris Neale

That sounds fair. The reason to use tips3p in place of tip3p is that Charmm36 lipid bilayers form a gel with tip3p and not with tips3p (I realize there are also other water models to try).

Just to provide a speed update, with gromacs 4.5.5 I find that tips3p runs at 85% of the speed of tip3p for a system of a protein in a POPC bilayer in water (box height=3 nm and either 5500/128 or 7000/166 water/POPC molecules). The charmm27 protein has each atom in its own charge group and I have attached the .mdp options below. I suppose the 85% vs. 50% could be due to the fact that half of the atoms in my system are not water atoms.

You can close this again, I just wanted to provide this information here.

Thank you,

Chris.

```
constraints = all-bonds
lincs-iter = 1
lincs-order = 6
constraint_algorithm = lincs
integrator = sd
dt = 0.002
tinit = 0
nstcomm = 1
nstlist = 10
ns_type = grid
vdwtype = switch
rist = 1.2
ristlong = 1.3
rvdw = 1.2
rvdw-switch = 0.8
rcoulomb = 1.2
coulombtype = PME
ewald-rtol = 1e-5
optimize_fft = yes
fourierspacing = 0.12
fourier_nx = 0
```

04/04/2020
This system would run much faster with the Verlet scheme. There the difference between tip3p and tips3p would only be around 5%. But I didn't implement a switch function yet. A plain cut-off of 1.1 nm might do a reasonable job. But it's scary that the phase behavior changes with water model, especially in the case where the worse water model performs better.

#4 - 07/15/2014 10:27 AM - Teemu Murtola

- Status changed from Closed to Rejected
- Target version deleted (future)