Gromacs - Bug #973

Energies from implicit solvent calculations

07/20/2012 06:18 PM - Geoffrey Wood

<table>
<thead>
<tr>
<th>Status:</th>
<th>Rejected</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
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<tr>
<td>Affected version - extra info:</td>
<td>Affected version: 4.5.3</td>
</tr>
</tbody>
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**Description**

Dear Developers,

I have recently been performing some test calculations for implicit solvent simulations and found what seems to be a discrepancy with the energies between the AMBER10 program package and the GROMACS 4.5.4 program package. The calculations I performed are very simple non-pbc minimizations of small TIP3P water clusters involving 1, 2, 4, and 8 molecules. To perform these in gromacs I first needed the GBSA parameters for TIP3P as these are by default undefined in gromacs. I took the parameters directly from my amber topologies and entered them in the gbsa.itp file after converting them from angstroms to nm, i.e.:

```plaintext
HW           0.1      1      1        0.120     0.85 ; H
OW           0.15     1      0.926    0.150     0.85 ; O
```

I then performed the implicit solvent minimizations in both gromacs and amber using the same GBSA model i.e. OBC with all parameters kept to their default values (which are the same default values in amber and gromacs) and compared the final energies. The results show that in each case the gromacs and amber energies are different by approximately a factor of 10:

<table>
<thead>
<tr>
<th></th>
<th>amber (kJ/mol)</th>
<th>gromacs (kJ/mol)</th>
<th>factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>water1</td>
<td>-48.44</td>
<td>-543.74</td>
<td>11.2</td>
</tr>
<tr>
<td>water2</td>
<td>-105.10</td>
<td>-1077.03</td>
<td>10.2</td>
</tr>
<tr>
<td>water4</td>
<td>-218.83</td>
<td>-2143.23</td>
<td>9.8</td>
</tr>
<tr>
<td>water8</td>
<td>-436.10</td>
<td>-4264.60</td>
<td>9.8</td>
</tr>
</tbody>
</table>

The literature value for the solvation energy of a single water molecule is approximately 46.0 kJ/mol indicating that the gromacs energies are too high by a factor of 10. After some initial investigations as to the origin of the discrepancy I believe there may be a unit conversion problem with the "sa_surface_tension" parameter. In KJ mol-1 nm-2 the default value for OBC model should be 2.25936 and in kcal/mol/ang^2 it should be 0.0054. The conversion factor between the two is involves a factor of 100 (ang^2 --> nm^2) and if this is under a square-root sign for GBSA this might result in the observed difference in energies by a factor of 10. I was wondering if any of the developers could help me confirm this or tell me if this is in fact an error on my part?

Please let me know if I need to provide any more information? As I said I performed the calculations with gromacs 4.5.4 on a standard 8 core (x86_64) unix box running centos 5 (kernal 2.6.18-164.6.1.el5). Gromacs was compiled with the gnu compilers (4.1.2) using autoconfig and linked to fftw3 (3.2.2).

Thanks in advance, Geoff Wood.

**Related issues:**

- Related to Gromacs - Feature #1292: mdrun features to deprecate for 5.0

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**History**

- #1 - 10/17/2012 10:19 PM - Roland Schulz
  - Status changed from New to Feedback wanted

I think the default sa_surface_tension value is correct. The documentation gives it as 0.0054 kcal/mol/Angstrom2 and the code (readir.c) uses "ir->sa_surface_tension = 0.0054 * CAL2JOULE * 100;". Am I mistaken or is that what you write it should be?
#2 - 01/11/2013 03:07 PM - Berk Hess
- Assignee changed from Berk Hess to Erik Lindahl

#3 - 01/09/2014 02:58 PM - Rossen Apostolov
- Affected version set to 4.5.3

Geoff, do you still see the same issue with the 4.6.x code?

#4 - 04/16/2014 01:48 PM - Rossen Apostolov
- Related to Feature #1292: mdrun features to deprecate for 5.0 added

#5 - 04/16/2014 01:49 PM - Rossen Apostolov
- Status changed from Feedback wanted to Rejected
- Assignee deleted (Erik Lindahl)

no further feedback from user, and GB will be deprecated anyway, thus closing