Gromacs - Bug #1134

gromacs 4.6 GB/SA problem and poor performance

01/27/2013 12:26 PM - Changwon Yang

Status: Closed
Priority: Normal
Assignee: Erik Lindahl
Category:

Target version: 4.6.x
Affected version:

extra info:
Affected version: 4.6

Description

I'm trying to run an md or em using an implicit solvation method using gromacs 4.6 but I always get the incorrect result.

ICC version : icc 11.0
fftw version : 3.2.2

Benchmark system is gromacs-gpubench
gromacs-gpubench-dhfr.tar/CPU/dhfr-impl-inf.bench

Angle, Proper Dih, Imp Dih, Nonpolar sol, LJ-14, Coulomb-14 energy are correct.
but GB polarization energy is too low, LJ, Coulomb(SR) energy are always zero.

It seems that there is a bug in the program.

Using gromacs 4.5. It works fine.

Gromacs 4.5.3 : 9.4ns/day
Gromacs 4.6 : 2.4ns/day

Input files: conf.gro and mdp files

http://www.gromacs.org/Documentation/Installation_Instructions_4.5/GROMACS-OpenMM


cpu-imp-RF-inf.mdp

constraints = all-bonds
integrator = md
dt = 0.002 ; ps !
nsteps = 0
nstlist = 0
ns_type = grid
rlist = 0
coulombtype = cut-off
vdwtype = cut-off
rcoulomb = 0
rvdw = 0
pbc = no
epsilon_rf = 0
rgbradii = 0
comm_mode = angular

implicit_solvent = GBSA
gb_algorithm = OBC
gb_epsilon_solvent = 78.3
sa_surface_tension = 2.25936

nstxout = 0
nstfout = 0
nstvout = 0

11/25/2015
gromacs 4.6 (icc 11.0, centos 5.8, fftw 3.2.2)

Statistics over 101 steps [ 0.0000 through 0.2000 ps ], 10 data sets
All statistics are over 11 points

<table>
<thead>
<tr>
<th>Energy</th>
<th>Average</th>
<th>Err.Est.</th>
<th>RMSD</th>
<th>Tot-Drift</th>
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<tbody>
<tr>
<td>Angle</td>
<td>4189.86</td>
<td>1094.25</td>
<td>2527.08</td>
<td>(kJ/mol)</td>
</tr>
<tr>
<td>Proper Dih.</td>
<td>6600.66</td>
<td>234.905</td>
<td>471.156</td>
<td>(kJ/mol)</td>
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<tr>
<td>Improper Dih.</td>
<td>121.598</td>
<td>32.7574</td>
<td>64.572</td>
<td>(kJ/mol)</td>
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<tr>
<td>GB Polarization</td>
<td>32708.8</td>
<td>1979.66</td>
<td>6416.79</td>
<td>(kJ/mol)</td>
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<tr>
<td>Nonpolar Sol.</td>
<td>158.323</td>
<td>13.0032</td>
<td>42.232</td>
<td>(kJ/mol)</td>
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<tr>
<td>LJ-14</td>
<td>2346.66</td>
<td>180.767</td>
<td>289.567</td>
<td>(kJ/mol)</td>
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<tr>
<td>Coulomb-14</td>
<td>26555.4</td>
<td>1091.98</td>
<td>3000.88</td>
<td>(kJ/mol)</td>
</tr>
<tr>
<td>LJ (SR)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(kJ/mol)</td>
</tr>
<tr>
<td>Coulomb (SR)</td>
<td>7263.71</td>
<td>1835.42</td>
<td>-6023.06</td>
<td>(kJ/mol)</td>
</tr>
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</table>

Related issues:
Related to Gromacs - Feature #1095: Fix all-vs-all kernels  In Progress 12/28/2012
Related to Gromacs - Bug #1249: no-PBC no-cutoff is broken with SIMD group... Closed 05/14/2013

History

#1 - 01/27/2013 09:13 PM - Changwon Yang
Using inf.cut-off, I always get the incorrect result. using finite cut-off, It works fine.(ICC version 13.0 or 11.0).

#2 - 06/26/2013 01:37 AM - Mark Abraham
- Target version set to 4.6.x
- Affected version set to 4.6

Thanks. This is a known bug. See http://redmine.gromacs.org/issues/1249. Setting GMX_NOOPTIMIZEDKERNELS gives correct results. The Verlet scheme also gives correct results.

#3 - 07/05/2013 06:34 PM - Mark Abraham
- Status changed from New to In Progress
- Assignee set to Erik Lindahl

#4 - 05/14/2014 10:54 AM - Rossen Apostolov
- Status changed from In Progress to Resolved

Closing that too

#5 - 05/23/2014 01:54 PM - Rossen Apostolov
- Status changed from Resolved to Closed

Files

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<tr>
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<th>Date</th>
<th>Author</th>
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<tr>
<td>topol.top</td>
<td>708 KB</td>
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<tr>
<td>cpu-imp-RF-inf.mdp</td>
<td>819 Bytes</td>
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<td>Changwon Yang</td>
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<td>01/27/2013</td>
<td>Changwon Yang</td>
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