

GROMACS - Bug #118

problem of g_energy -nmol

11/10/2006 08:28 AM - qiaobf empty

Status:	Closed	Difficulty:	uncategorized
Priority:	High		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	3.3.1		
Affected version - extra info:			
Affected version:			

Description

When using the g_energy -nmol to calculate the energy, only the Bond, Angle, Potential terms are right, while the LJ, Coulomb, Total-Energy give the same value as without -nmol.

See the following two tests.

Test 1.

g_energy -f md3.edr

Energy	Average	RMSD	Fluct.	Drift	Tot-Drift
Bond	1370.47	64.952	64.8116	0.0295732	14.7866
Angle	3541.69	99.9164	99.9059	0.0100593	5.02964
LJ-(SR)	3601.66	151.232	131.574	0.516572	258.287
Coulomb(SR)	-10883	143.406	134.139	-0.351347	-175.674
Potential	-30962.9	304.081	265.607	-1.0257	-512.85
Total-Energy	-22436.1	287.863	245.635	-1.03989	-519.945

g_energy -nmol 115 -f md3.edr

Energy	Average	RMSD	Fluct.	Drift	Tot-Drift
Bond	11.9171	0.5648	0	0.0295732	14.7866
Angle	30.7973	0.868838	0	0.0100593	5.02964
LJ-(SR)	3601.66	151.232	131.574	0.516572	258.287
Coulomb(SR)	-10883	143.406	134.139	-0.351347	-175.674
Potential	-269.242	2.64418	0	-1.0257	-512.85
Total-Energy	-22436.1	287.863	245.635	-1.03989	-519.945

Test 2.

g_energy -f md3.edr

Energy	Average	RMSD	Fluct.	Drift	Tot-Drift
Bond	27255.4	288.517	287.731	0.147486	73.7433
Angle	30206.8	299.196	299.151	0.0361126	18.0563
LJ(SR)	27021.1	1153.88	1015.89	3.7911	1895.55
Coulomb(SR)	-116585	1327.11	1120.39	-4.92805	-2464.03
Potential	-271448	2889.94	2444.54	-10.6792	-5339.61
Total-Energy	-183054	2912.13	2478.91	-10.588	-5293.99

g_energy -nmol 981 -f md3.edr

Energy	Average	RMSD	Fluct.	Drift	Tot-Drift
Bond	27.7833	0.294105	0	0.147486	73.7433

Angle	30.7919	0.304991	0	0.0361126	18.0563
LJ(SR)	27021.1	1153.88	1015.89	3.7911	1895.55
Coulomb(SR)	-116585	1327.11	1120.39	-4.92805	-2464.03
Potential	-276.705	2.94591	0	-10.6792	-5339.61
Total-Energy	-183054	2912.13	2478.91	-10.588	-5293.99

History

#1 - 12/23/2006 04:52 PM - David van der Spoel

This is a duplicate of bug 76 which was fixed already in CVS.