ReadMe

Improved angle potentials for coarse-grained molecular dynamics simulations

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To improve the stability and accuracy of coarse-grained molecular dynamics simulations we introduced new angle potentials:[1]

1. restricted bending (ReB) potential,

$$V_{\mathrm{ReB}}(\theta_i) = \frac{1}{2}k_\theta \frac{(\cos\theta_i - \cos\theta_0)^2}{\sin^2\theta_i}, \tag{1}$$

   prevents torsion angles from visiting unstable or unphysical configurations

2. combined bending-torsion (CBT) potential,

$$V_{\mathrm{CBT}}(\theta_{i-1}, \theta_i, \phi_i) = k_\phi \sin^3\theta_{i-1} \sin^3\theta_i \sum_{n=0}^{4} a_n \cos^n\phi_i, \tag{2}$$

   smoothly flattens the interactions when such configurations are sampled.

3. restricted torsion (ReT) potential,

$$V_{\mathrm{ReT}}(\phi_i) = \frac{1}{2}k_\phi \frac{(\cos\phi_i - \cos\phi_0)^2}{\sin^2\phi_i}, \tag{3}$$

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keeps the torsion angle at only one minimum value.

These angle potentials have been implemented into an *in-house* version of Gromacs (gromacs_4.0.7_torsion), publicly available on the MARTINI web-page (http://cgmartini.nl). They will be part of the regular next Gromacs release. Table 1 shows the three potentials with the corresponding input parameters needed in the topology files (.itp) describing the molecular interactions.

Table 1: Gromacs definitions of the intramolecular interaction concerning the modified potentials. The function type and parameters are conform with the Gromacs definition. *The function type may differ in the next Gromacs release.

Interaction type	directive	# at.	f* tp	parameters
ReB	angles	3	9	θ_0, k_θ
ReT	dihedrals	4	10	ϕ_0, k_ϕ
CBT	dihedrals	4	11	k_ϕ, a_0, a_1, a_2, a_3, a_4

Extra subroutines have been included into the original Gromacs "bondfree.c" subroutine to calculate the dihedral angle (its cosine and the contributions of the torsion force on each particle forming the dihedral). Additionally, the *input-output* and the preprocessing subroutines have been modified to read / write the new molecular topology files and to create the binary topology file (.tpr) for the MD run. The utilities *mk_angndx* and *g_angle* have been also extended to describe and calculate the new types of angles.

The new angle potentials can be tested on simulations of an ensemble of polyethylene glycol (PEG) chains in water, at low density. In the original PEG model (PEG-OR) a cosine-harmonic function is used for the bending potential, and a combination of four torsion potentials for the dihedral angle[2] (see the parameters in Table 2).

To perform simulations with the new angle potentials, two sets of files can be downloaded from the MARTINI web-page (http://cgmartini.nl) - one for PEG-ReB (*peg_ReB.itp*, *peg_ReB.top*) and one for PEG-CBT (*peg_CBT.itp*, *peg_CBT.top*). The *peg.gro*, *peg.mdp* and *martini_v2.0.itp* are common files.

Table 2: The angle potentials used in the PEG simulations: the type, the reference angle and the optimum interaction parameters.

	BENDING			TORSION			
	type	θ_0 [deg]	k_B [kJ mol^{-1}]	type	ϕ_0 [deg]	k_ϕ [kJ mol^{-1}]	n / a_i
PEG-OR	2	130	85	1	180	1.96	1
				1	0	0.18	2
				1	0	0.33	3
				1	0	0.12	4
PEG-ReB	2	130	50	idem			
	9	130	25				
PEG-CBT	2	116	110	10	–	10	$a_0 = 2.41$
							$a_1 = -2.95$
							$a_2 = 0.36$
							$a_3 = 1.33$
							$a_4 = 0.00$

References

(1) Bulacu, M.; Goga, N.; Zhao, W.; Rossi, G.; Monticelli, L.; Periole, X.; Tieleman, D. P.; Marrink, S. J. *Journal of Chemical Theory and Computation, in press*.

(2) Lee, H.; de Vries, A. H.; Marrink, S.-J.; Pastor, R. W. *J. Phys. Chem. B* **2009**, *113*, 13186–13194.