Electronic supplementary information (ESI)

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1 Tabulated potentials

Coarse-grained bonded and nonbonded potentials that have been discussed in the main text are reported in additional files with .pdf extension. The tabulated CG potentials are stored in CG1.pdf, CG2.pdf, CG3.pdf, CG4.pdf, CG4*.pdf, covering the different resolution that have been considered in the article.

Details concerning the tabulation of the potentials, such as the range of the tabulated values and the discretization criteria, are presented in Table 1. Distances are given in Å, angles in degrees and energies in kcal/mol.

Degree of freedom	Initial value	Final value	Step size		
r_b (Å)	0.01	5.00 or 6.00	0.01		
heta (°)	0.00	180.00	0.5		
arphi (°)	-180.00	180.00	0.5		
r_{nb} (Å)	0.01	11.00	0.01		

Table 1: Discretization of the potentials in tabular form

2 CRW potentials for CG4 mapping scheme

CRW potentials developed when grouping four carbons and connected hydrogens in a single bead are shown in Figure 1. CG4 potential has been derived under no specific assumption, using L-OPLS dihedral description. For CG4^{*} one of the dihedrals of the

molecules has been constrained to the gauche configuration, while for $CG4^{**}$ both dihedrals are blocked at ~60° during the sampling. The constrained dihedrals runs are considered with the aim of recovering the correct gauche-trans distribution during the sampling performed to derive the nonbonded interaction. In the main text the features of the potentials and their performance are discussed. In Figure 2 is shown the improvement of the radial distribution function when using the CG4* set of potentials over the CG4 force field.

$3 \quad g(r)$ for tabulated and analytical potentials

By fitting the tabulated nonbonded potentials onto Mie functions, an additional group of potentials is generated for each level of resolution. The two set of potentials are similar but not equivalent. As shown in Figure 9 in the main text, small deviations are observed in the repulsive region and as far as the depth of the minima is concerned. Here, the radial distribution functions of the center of mass of n-dodecane, for atomistic, CG tabulated and CG analytical potentials are shown (Figure 3). A good agreement is achieved between RDFs computed using Mie potentials or their original tabulated form.

4 Speed up of the CG models

The coarse-graining process leads to a reduction of the number of interaction sites and to an acceleration of the computation times. At the CG level the electrostatic interactions are, in our case, not considered, which also contributes to the speed up. In Table 2, CPU times are listed for 0.5 ns MD runs on a single processor and for 10 ns parallel runs on 24 processors for the atomistic and CG systems. The MD simulations are performed on AMD Opteron 6174 processors. Already for CG1 the calculation is more than one order of magnitude faster and the further the system is simplified, the faster the computation goes.

Coarse-grained simulation display faster dynamics due to softening of the interactions.

In order to assess the dynamic speed up achieved we calculate the ratio between CG and atomistic diffusion coefficient, $S = \frac{D_{CG}}{D_{AA}}$. The diffusion coefficient of the center of mass of n-dodecane is computed in the linear region of the mean squared displacement. The speed-up factor S and the diffusion coefficient are reported for each system in Table 3. It is possible to notice how the diffusion behaviour of CG1 model is close to the atomistic one. In fact, united-atom models in which hydrogens are grouped to the connected heavy atom are closely-related to fully atomistic description also from the dynamic point of view.

	1-processor	1-processor 24-processors	
	(0.5 ns run)	(10 ns run)	
L-OPLS	43.98	58.04	
CG1	2.06	3.05	
CG2	0.52	1.17	
CG3	0.27	1.12	
CG4*	0.18	0.79	

Table 2: CPU cost of atomistic and coarse-grained dynamics (n-dodecane, 200 molecules)expressed in CPU-hours

Table 3: Diffusion coefficient and speed up factor S

	D $(10^{-5}cm^2s^{-1})$	\mathbf{S}
L-OPLS	0.65	-
CG1	0.78	1.20
CG2	3.02	4.65
CG3	2.45	3.77
$CG4^*$	2.98	4.58



Figure 1: Comparison of different potentials developed for the same mapping scheme (four heavy atoms mapped on a single site).



Figure 2: Radial distribution functions of the center of mass (upper panel) and with respect to the different bead types (lower panel). A black continuous line is used for the atomistic results, CG4 data are shown with a blue dashed line and CG4* with a red dashed line.



Figure 3: Radial distribution functions for the center of mass of n-dodecane. Tabulated (blue line) and analytical potentials (red line) perform comparatively well. The atomistic reference is plotted with black continuous line.