

Coarse-graining

“reducing the irrelevant degrees of freedom”



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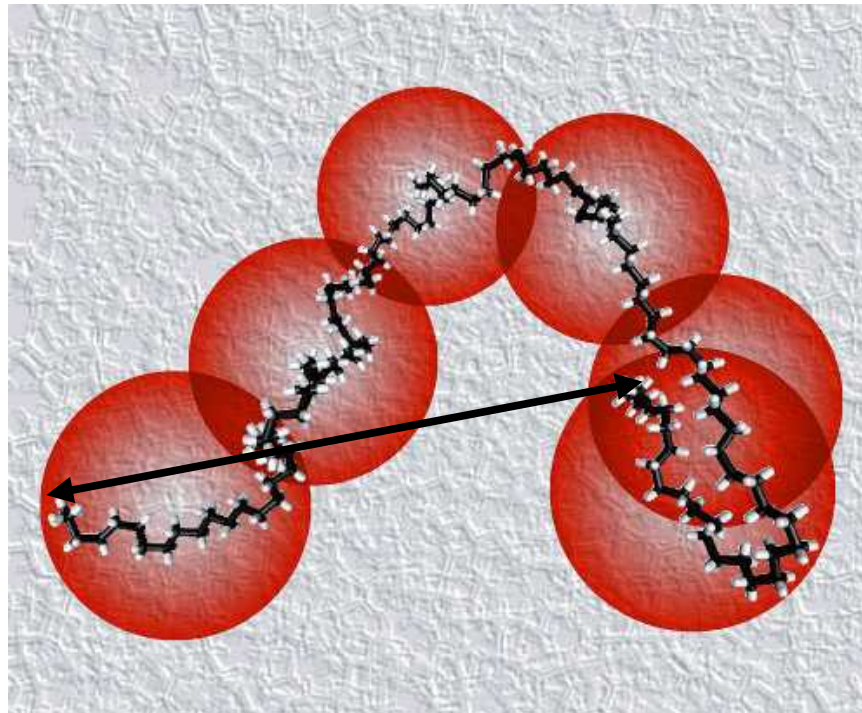
Compressed to 24Kb

The 'coarse-grained' picture is poor resolution. Yet, the sea, rock, trees and clouds is still recognizable. In fact, on 5 m distance from the screen it is hard to tell the difference between the two pictures.

Goal of Coarse-Graining (CG)

Goal: Scale up the size and time-scale of a fine-grained system of interest via the reduction of irrelevant degrees of freedom.

Coarse-grained simulations are commonly used for studying polymers, granular mater, colloids and biological materials!



Example: How does the end-to-end distance of a polymer in solution changes with polymer length?

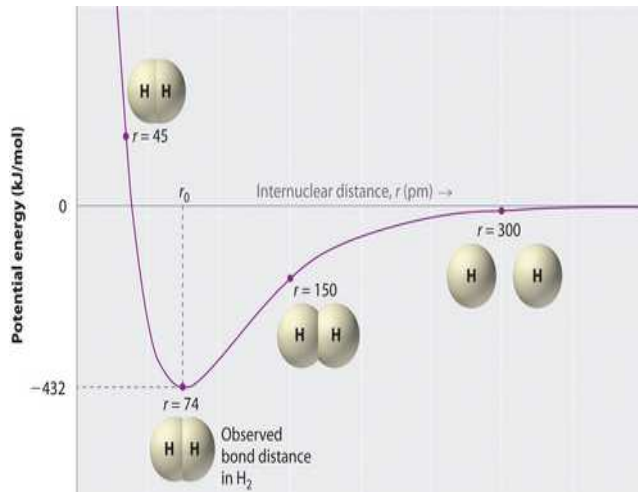
Problem: Fine-grained (atomistic) simulations can only yield limited data points.

Solution: Construct a coarse-grained model.

Coarse-graining

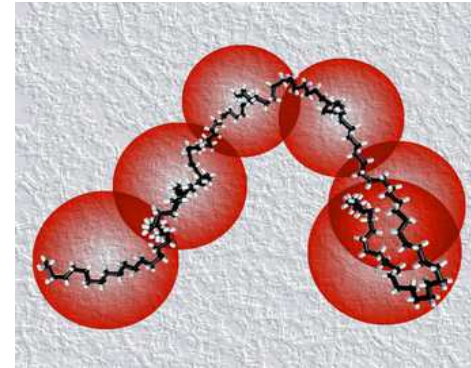
“reducing the irrelevant degrees of freedom”

'Classic' atomic description:
bead size = van der Waals radius

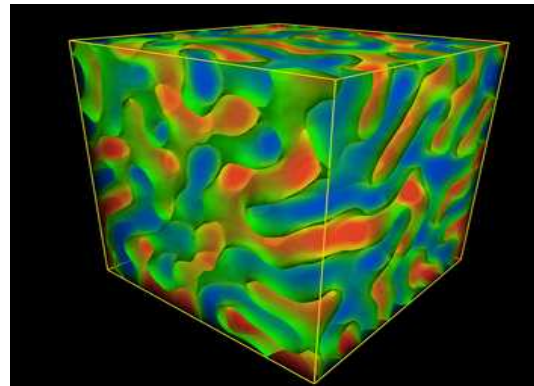


$$U_{AA} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \alpha \left(\frac{\sigma}{r} \right)^6 \right]$$

Coarse-grained description:

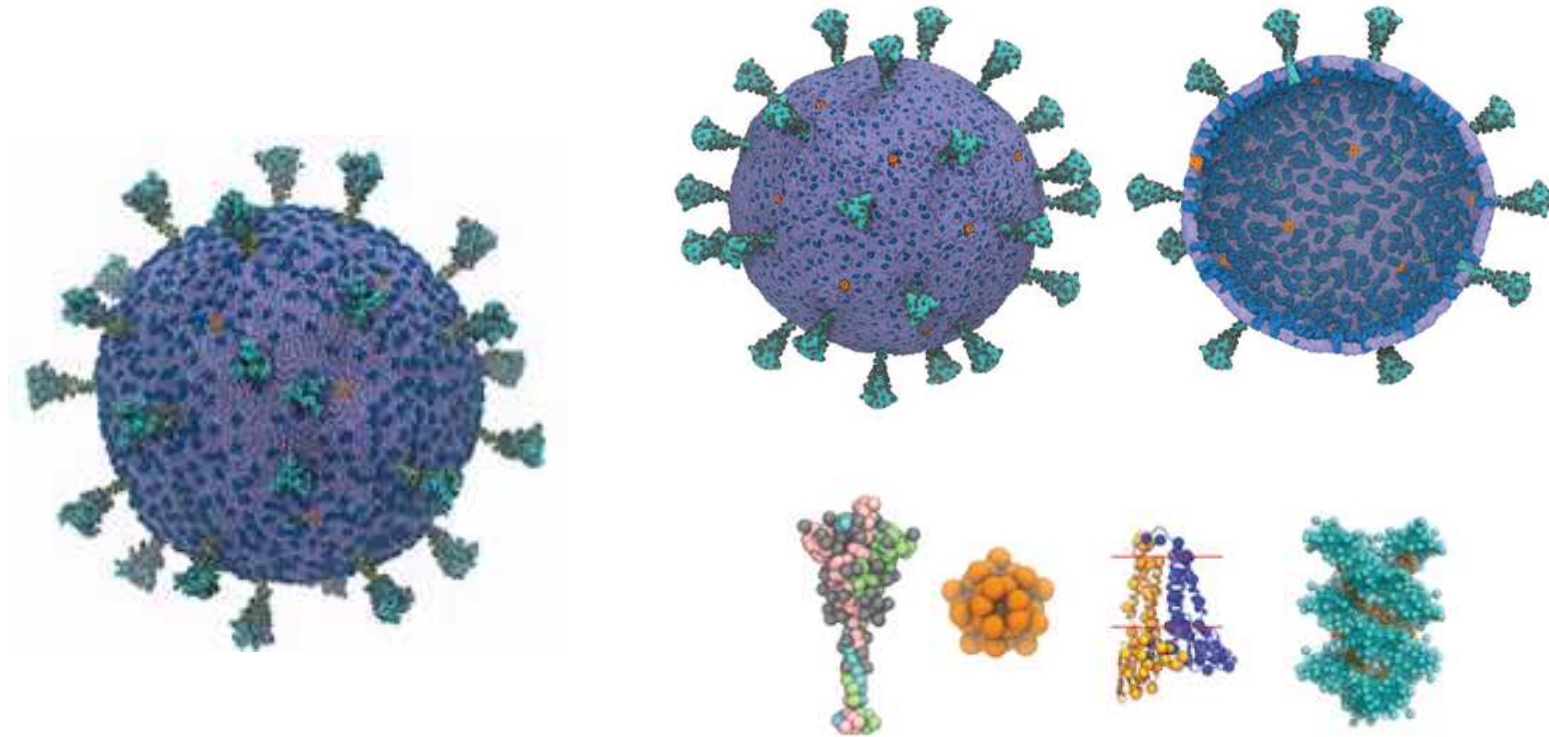


- particle based description
- allows larger Δt , results in faster diffusion (irrelevant degrees → friction)



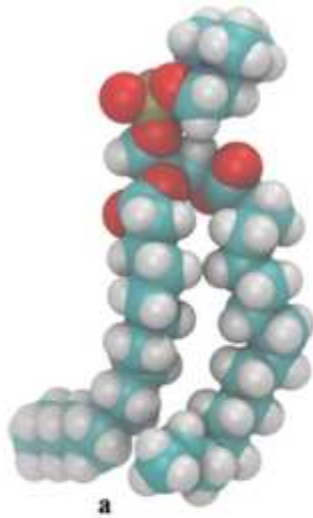
- density based description
- diffusion equations

Coarse-graining: SARS-COV2 virus

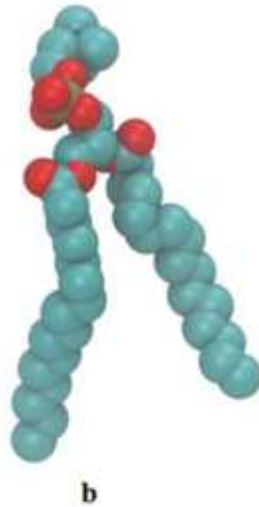


Voth group, Uchicago
CG method: force matching

Coarse-graining: A lipid



All-atom model
118 atoms



United-atom
model:
46 united atoms



Coarse-grained
10 sites:
Martini model



Coarse-grained
3 sites:
Cooke model

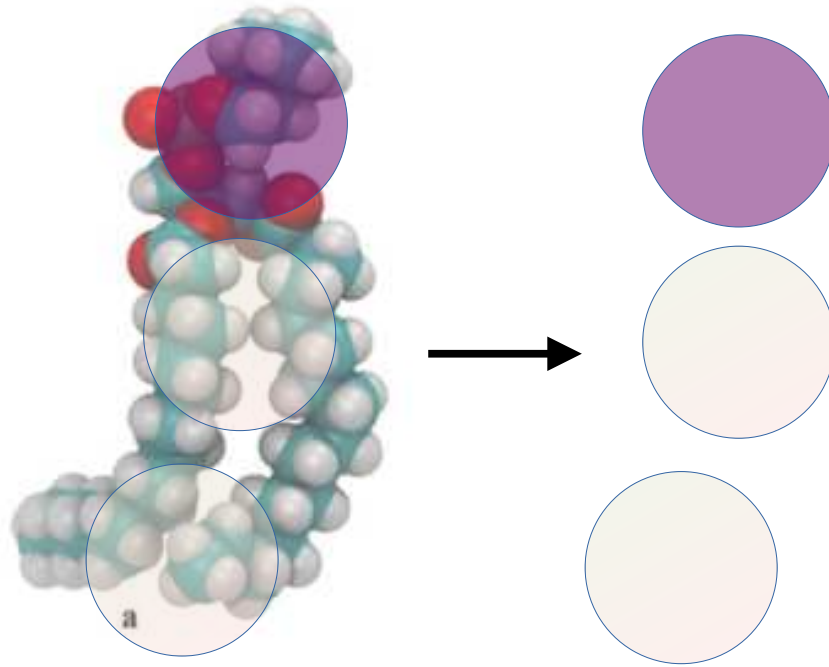
← more details - chemical specificity

faster computations; larger systems →

Goarse-graining: General idea

{ indicate a single specific configuration

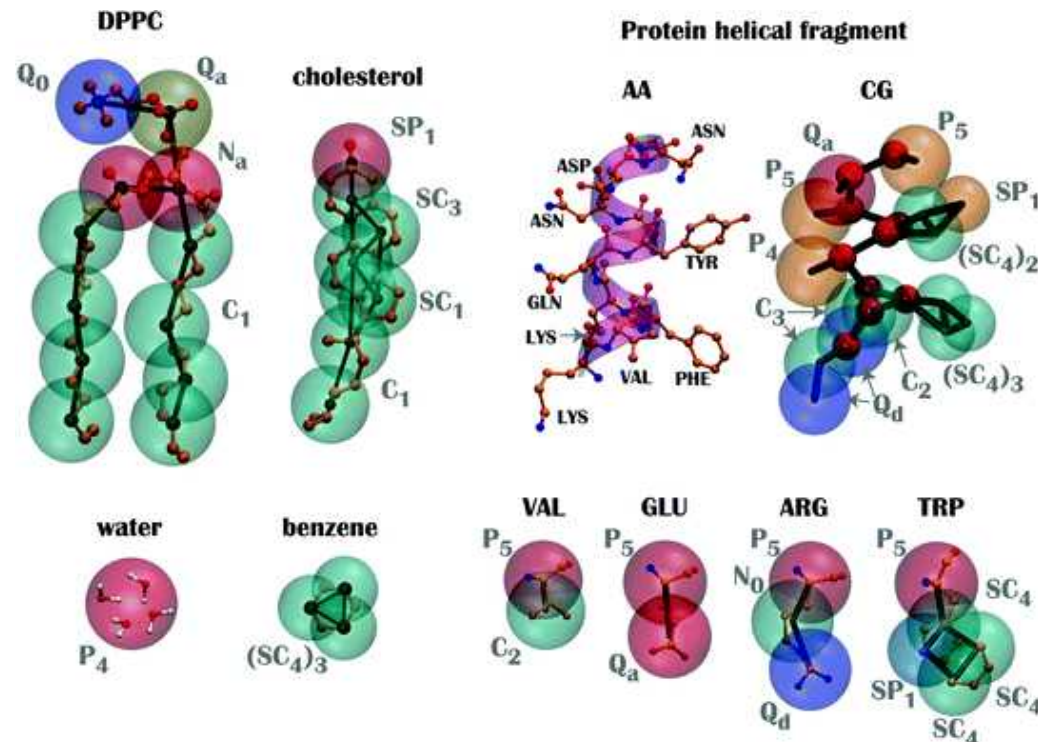
$$\mathcal{M} : \{r\} \rightarrow \{R\}$$



Goarse-graining: Example of a mapping scheme (the Martini model)

{ } indicate a single specific configuration

$$\mathcal{M} : \{r\} \rightarrow \{R\}$$



Marrink, Risselada,...,Mark, J. Phys. Chem. B, 2007

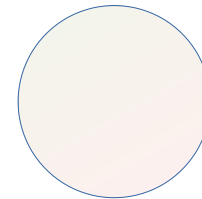
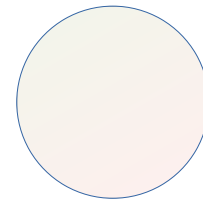
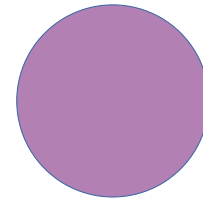
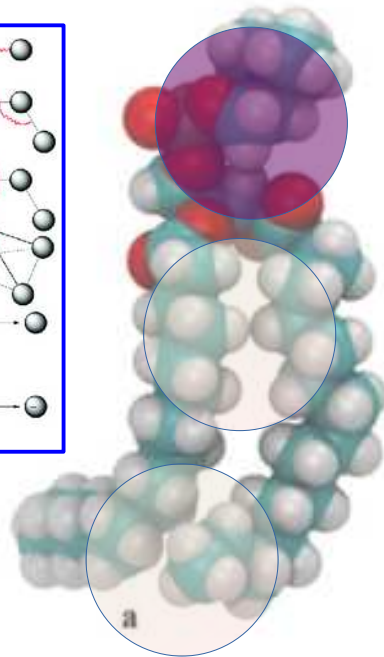
The mapping is predefined or better user-defined!

Goarse-graining: What to solve...

$\{$ indicate a single specific configuration

$$\mathcal{M} : \{r\} \rightarrow \{R\}$$

$$\begin{aligned}
 U(R) = & \sum_{\text{bonds}} k_r (r - r_{eq})^2 & \text{bond} \\
 & + \sum_{\text{angles}} k_\theta (\theta - \theta_{eq})^2 & \text{angle} \\
 & + \sum_{\text{dihedrals}} k_\phi (1 + \cos[n\phi - \gamma]) & \text{dihedral} \\
 & + \sum_{\text{impropers}} k_\omega (\omega - \omega_{eq})^2 & \text{improper} \\
 & + \sum_{i < j}^{\text{atoms}} \epsilon_{ij} \left[\left(\frac{r_m}{r_{ij}} \right)^{12} - 2 \left(\frac{r_m}{r_{ij}} \right)^6 \right] & \text{van der Waals} \\
 & + \sum_{i < j}^{\text{atoms}} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} & \text{electrostatic}
 \end{aligned}$$

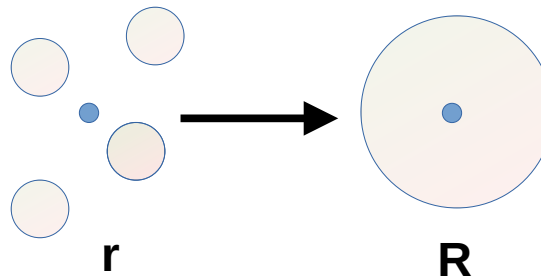
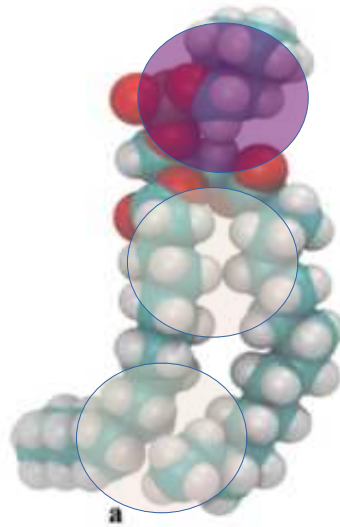


?

- Given the defined mapping \mathbf{M} , how would the corresponding CG force-field or Hamiltonian look like?

Coarse-graining: Fundamentals

- For each coarse-grained configuration \mathbf{R} there exists a sub-ensemble of fine-grained configurations \mathbf{r} . Therefore, only the mapping from \mathbf{r} to \mathbf{R} is well-defined!



Goarse-graining: General idea

- The mapping operation **M** only acts on the configuration space.

$$\mathcal{M} : \{r\} \rightarrow \{R\}$$

- The goal of coarse-graining is to reproduce the configurational part of the fine-grained partition function Z_0 for all relevant degrees of freedom while omitting all irrelevant degrees of freedom:

$$Z_0 = \int d\{r\} e^{-\beta H_0}$$

Goarse-graining: General idea

- The coarse-grained partition function can be expressed in terms of the original fine-grained Hamiltonian :

$$Z_{CG} = \int d\{R\} e^{-\beta H_{CG}} = \int d\{R\} \int d\{r\} \delta(R - \mathcal{M}(r)) e^{-\beta H_0(\{r\})}$$

$$Z_{CG} = \int d\{r\} e^{-\beta H_0(\{r\})} = Z_0$$

- Constructing all coarse-grained configurations from all fine-grained configurations:

$$\Omega(\{R\}) \rightarrow \int d\{r\} \delta(R - \mathcal{M}(\{r\}))$$

Goarse-graining: General idea

- Coarse-graining poses an inverse problem: We can construct all the configurations R from the fine-grained trajectory r , since we know the mapping \mathbf{M} . Therefore, we can in principle reconstruct H_{CG} since H_0 is known.

$$Z_{CG} = \int \underbrace{d\{R\}}_{\text{unknown!}} e^{-\beta H_{CG}} = \int d\{R\} \int \underbrace{d\{r\} \delta(R - \mathcal{M}(r)) e^{-\beta H_0(\{r\})}}_{\text{known}}$$

- Disclaimer:** U_{CG} is only solved for a particular thermodynamic state point corresponding to the fine-grained ensemble/trajectory (temperature and pressure).
The solution for U_{CG} is therefore not generally transferable to other state points!

Goarse-graining: Henderson theorem

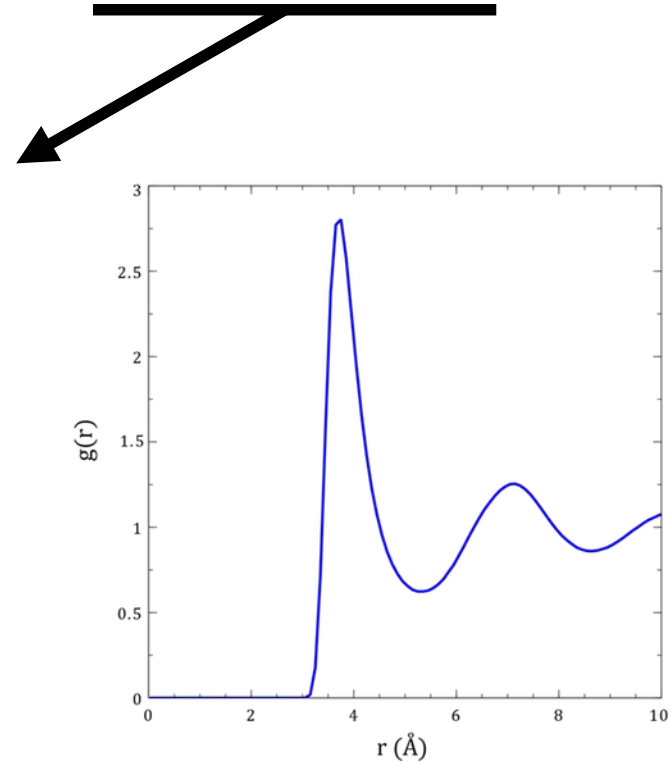
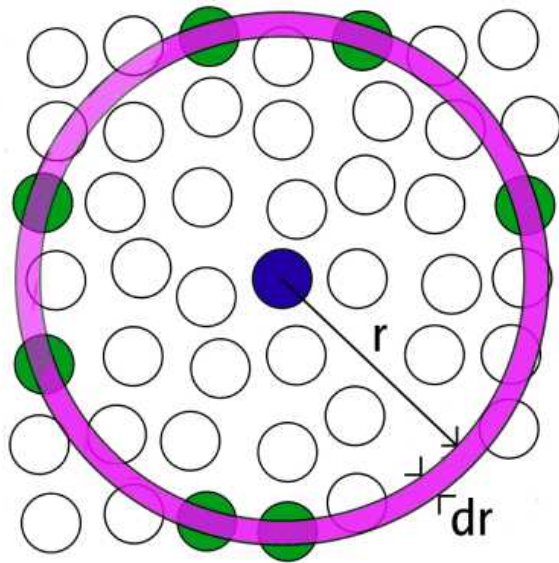
Formulate structure based on correlation functions:

	$\rho_1(\mathbf{r}_1)$	density
All we use! →	$\rho_2(\mathbf{r}_1, \mathbf{r}_2)$	pair correlation, RDF or $g(r)$
	$\rho_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$	3-body correlation

Henderson theorem: “For each set of RDFs there is an unique set of pair potentials reproducing this set of RDFs” (R.L.Henderson, Phys. Lett. A., 1974). In essence, this theorem is analogous to the Kirkwood superposition approximation (!) stating that multibody correlations can be effectively decomposed into pair correlations (RISM integral theory).

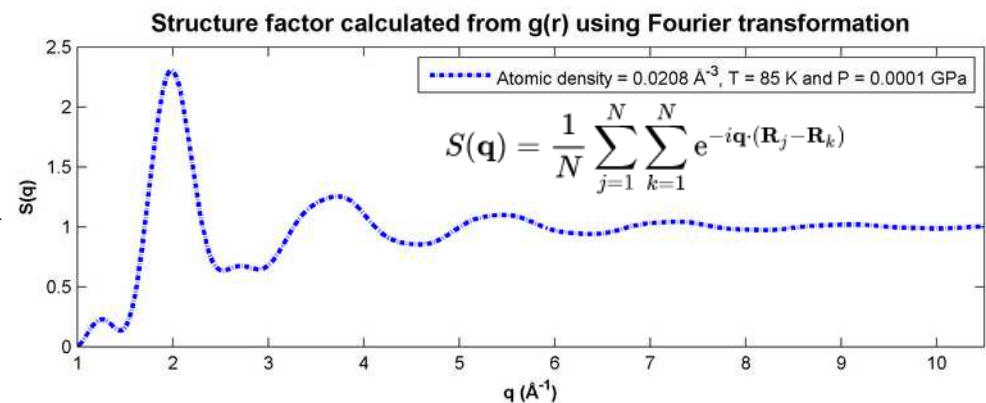
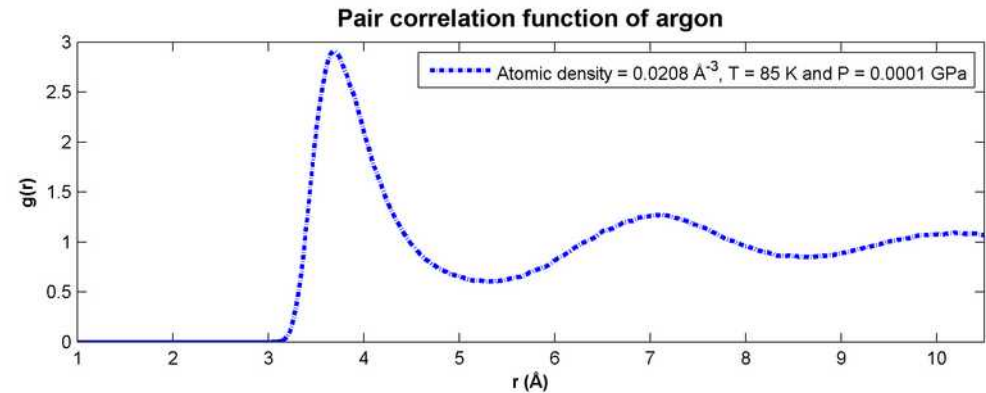
Systematic coarse-graining: Structure based

$$Z_{CG} = \int d\{R\} e^{-\beta H_{CG}} = \int d\{R\} \int d\{r\} \delta(R - \mathcal{M}(r)) e^{-\beta H_0(\{r\})}$$



$$g(r) = \frac{V}{4\pi r^2 N^2} \left\langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \right\rangle$$

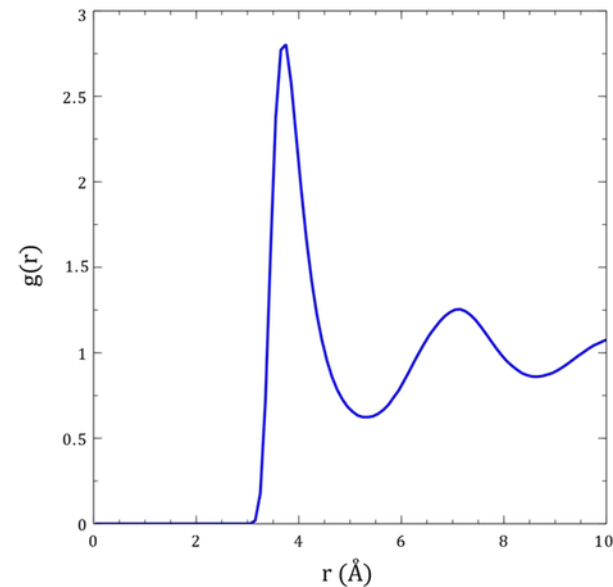
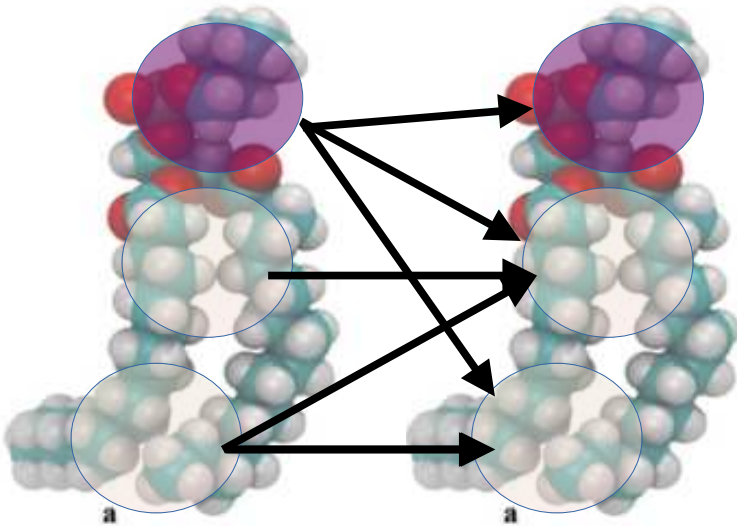
Systematic coarse-graining: Structure based



- The fourier transform of $g(r)$ – the structure factor $S(q)$ – can be experimentally resolved by Xray and neutron scattering.

Systematic coarse-graining: Structure based

$$Z_{CG} = \int d\{R\} e^{-\beta H_{CG}} = \int d\{R\} \int d\{r\} \delta(R - \mathcal{M}(r)) e^{-\beta H_0(\{r\})}$$



- If there are n unique bead types, then $n!$ different $g(r)$ must be reproduced for the non-bonded interactions!
- For the bonded interactions bond length and angle distributions must be (simultaneously) reproduced!

Systematic coarse-graining: Structure based

$$Z_{CG} = \int d\{R\} e^{-\beta H_{CG}} = \int d\{R\} \int d\{r\} \underbrace{\delta(R - \mathcal{M}(r))}_{\text{known}} e^{-\beta H_0(\{r\})}$$

Solve!

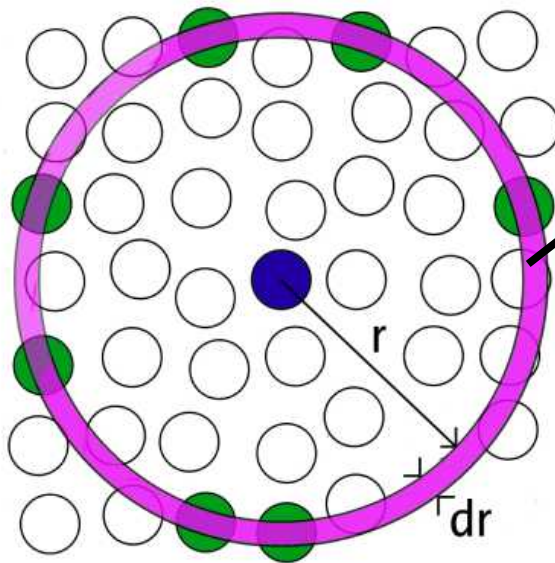
Two main approaches for structured-based systematic coarse-graining:

- 1) Inverse Monte-Carlo.
 - 2) Inverse Boltzman.
- Both IMC and IB rely on iterative adaptation/fitting of a tabulated trial potential to reproduce $g^*(r)$.

Systematic coarse-graining: Inverse Monte-Carlo

$$Z_{CG} = \int d\{R\} e^{-\beta H_{CG}} = \int d\{R\} \int d\{r\} \underbrace{\delta(R - \mathcal{M}(r)) e^{-\beta H_0(\{r\})}}_{\text{known}}$$

Solve!



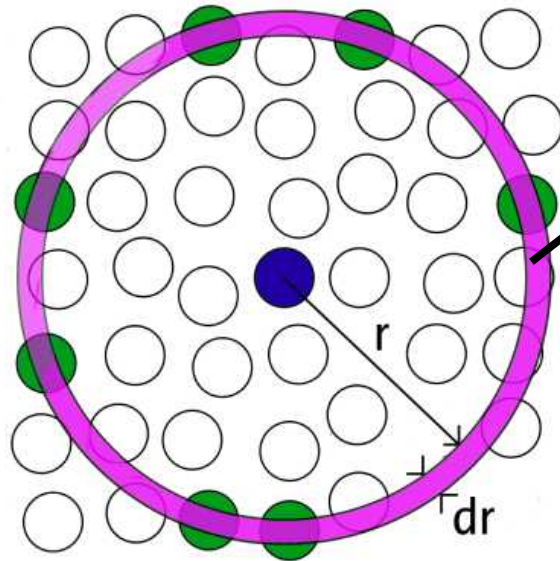
S_α The number of interaction pairs in the shell α (7 in this example).

The total energy is thus given by:

$$H = \sum_{\alpha} V_{\alpha} S_{\alpha}$$

unknown!

Systematic coarse-graining: Inverse Monte-Carlo



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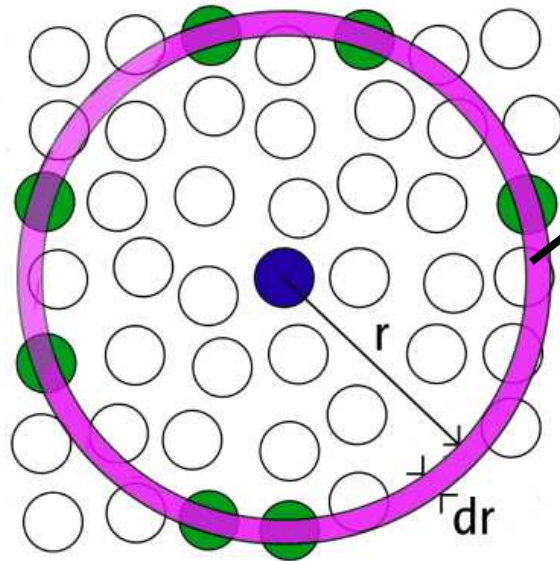
unknown!

Main idea: Construct a relationship between V and $\langle S \rangle$ or better its fluctuation $\Delta \langle S \rangle$:

$$\Delta \langle S_{\alpha} \rangle = \sum_{\gamma} \frac{\partial \langle S_{\alpha} \rangle}{\partial V_{\gamma}} \Delta V_{\gamma} + \mathcal{O}(\Delta V^2)$$

\swarrow
 coupling with the change in V in other shells!

Systematic coarse-graining: Inverse Monte-Carlo



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coupling with $\langle V \rangle$ in other shells!

Systematic coarse-graining: Inverse Monte-Carlo

Main idea: Construct a relationship between V and $\langle S \rangle$ or better its fluctuation $\Delta \langle S \rangle$:

$$\underbrace{\Delta \langle S_\alpha \rangle}_{\text{ensemble averaging}} = \sum_{\gamma} \left(\frac{\partial \langle S_\alpha \rangle}{\partial V_\gamma} \right) \Delta V_\gamma + \mathcal{O}(\Delta V^2)$$

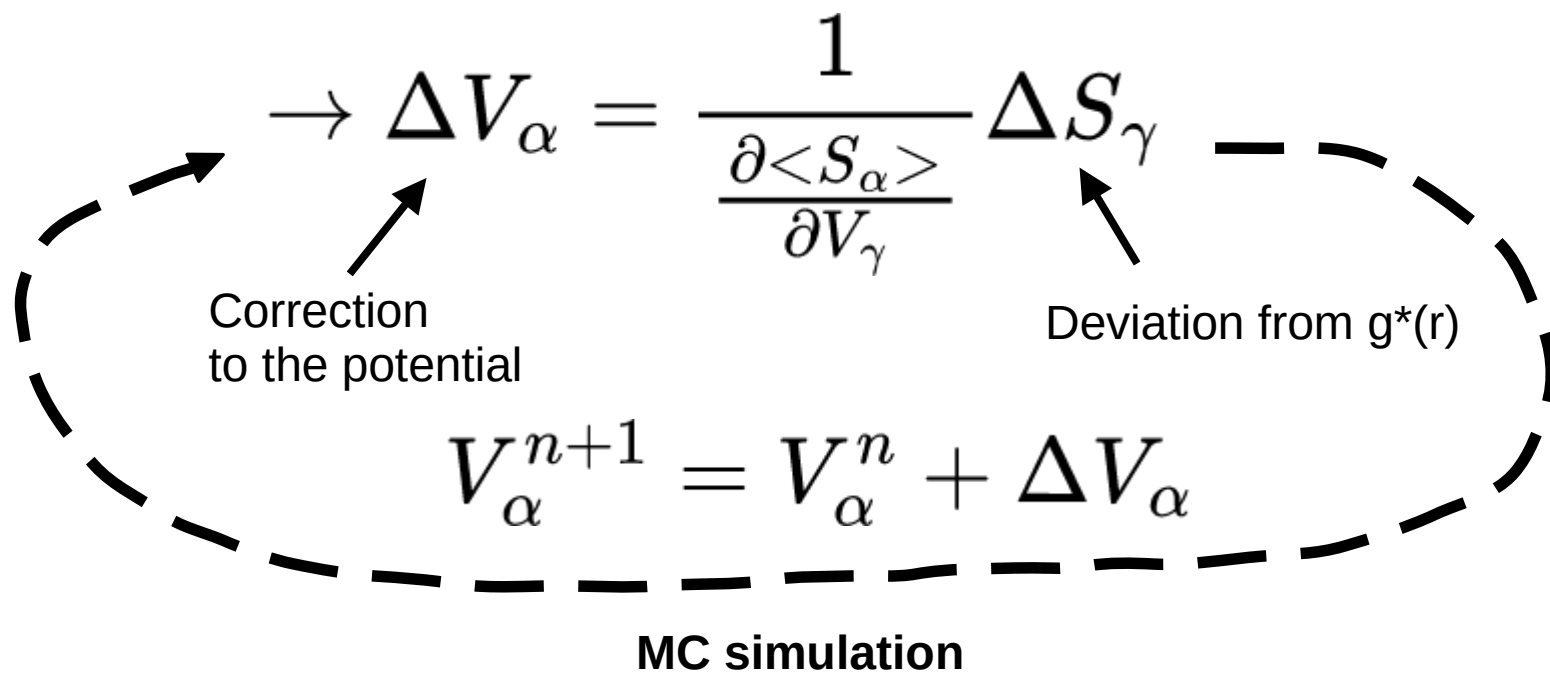
Accumulation yields ΔV at α .
Subsequent accumulation of $\Delta V(\alpha)$ yields $V(\alpha)$

$$\frac{\partial \langle S_\alpha \rangle}{\partial V_\gamma} = -\beta \underbrace{(\langle S_\alpha S_\gamma \rangle - \langle S_\alpha \rangle \langle S_\gamma \rangle)}_{\text{ensemble averaging}}$$

- Note that $V(\alpha)$ is a discrete potential! Forces are thus not well-defined! This is why Monte-Carlo is used rather than molecular dynamics to sample configurations.

Systematic coarse-graining: Inverse Monte-Carlo

$$\frac{\partial \langle S_\alpha \rangle}{\partial V_\gamma} = -\beta \underbrace{(\langle S_\alpha S_\gamma \rangle - \langle S_\alpha \rangle \langle S_\gamma \rangle)}_{\text{ensemble averaging}}$$



The diagram illustrates the iterative process of systematic coarse-graining. A dashed oval encloses the core simulation loop. At the top, the equation $\rightarrow \Delta V_\alpha = \frac{1}{\frac{\partial \langle S_\alpha \rangle}{\partial V_\gamma}} \Delta S_\gamma$ is shown. An arrow points from the text "Correction to the potential" to ΔV_α , and another arrow points from "Deviation from $g^*(r)$ " to ΔS_γ . Below this, the update equation $V_\alpha^{n+1} = V_\alpha^n + \Delta V_\alpha$ is displayed. The entire loop is labeled "MC simulation" at the bottom.

$$\rightarrow \Delta V_\alpha = \frac{1}{\frac{\partial \langle S_\alpha \rangle}{\partial V_\gamma}} \Delta S_\gamma$$

Correction to the potential

Deviation from $g^*(r)$

$$V_\alpha^{n+1} = V_\alpha^n + \Delta V_\alpha$$

MC simulation

Systematic coarse-graining: Inverse Monte-Carlo

Lyubartsev AP, Laaksonen A. *Calculation of effective interaction potentials from radial distribution functions: A reverse Monte Carlo approach*. Phys Rev E Stat Phys Plasmas Fluids Relat Interdiscip Topics. 1995

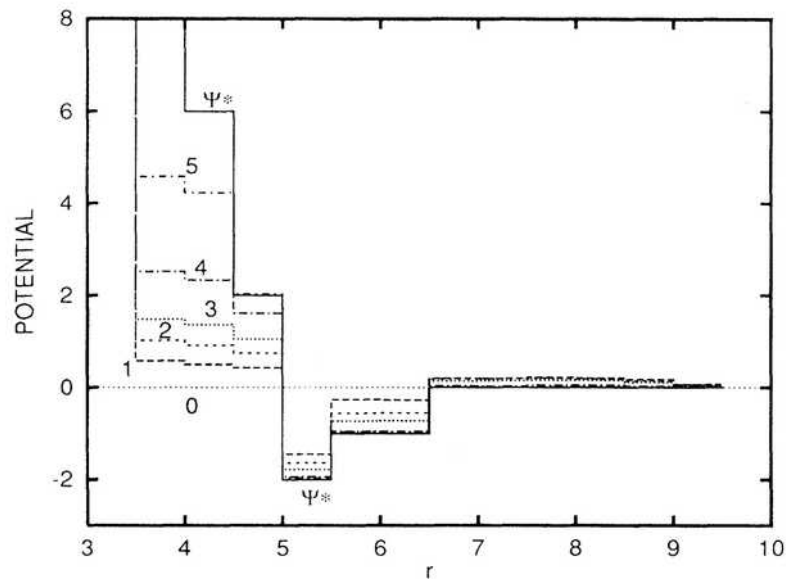
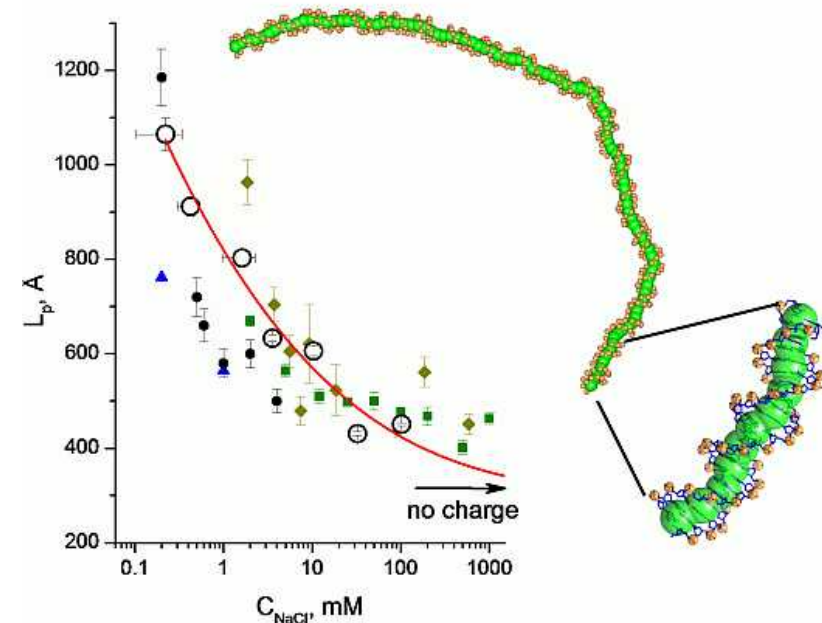


FIG. 2. An example of the convergent iterative procedure starting from zero potential with a damping parameter $\lambda=0.5$; notations as in Fig. 1.

Korolev, N., Luo, D., Lyubartsev, A. P., & Nordenskiöld, L. (2014). A Coarse-Grained DNA Model Parameterized from Atomistic Simulations by Inverse Monte Carlo. Polymers, 6(6), 1655-1675



- Potentials resolved with the Inverse Monte-Carlo method can be fitted to cubic splines and used for molecular simulations.

Systematic coarse-graining: Inverse Boltzmann

Update $V(r)$ using a simple iterative scheme in MD simulations:

$$\Delta V^n(r) = k_B T \ln(g^n(r)/g^*(r))$$

The value of the potential $V(r)$ at r is obtained via accumulation of all ΔV s upto r :

$$V(r) = \Delta V(\alpha) + \Delta V(\beta) \dots$$

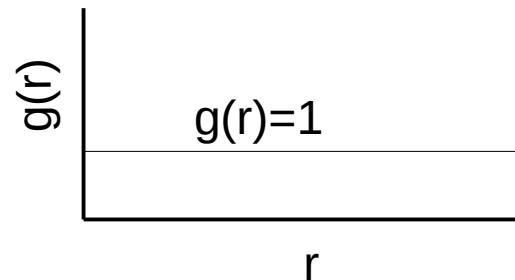
Schommers, Phys. Rev. A, 28, 3599 (1983)
D. Reith et al., J. Chomp. Chem. 24(13), 1624 (2003)
A. Lyubartsev et al., Phys. Rev. E. 52 (4), 3730 (1995)

- $V(r)$ must be fitted to cubic splines after each iteration n if based on MD!
- May yield a different result than IMC.
- May not completely convert in case of multicomponents (multi-objectives).

Systematic coarse-graining: Inverse Boltzmann

$$\Delta V^n(r) = k_B T \ln(g^n(r)/g^*(r))$$

Initial 'guess' : $g(r)=1$



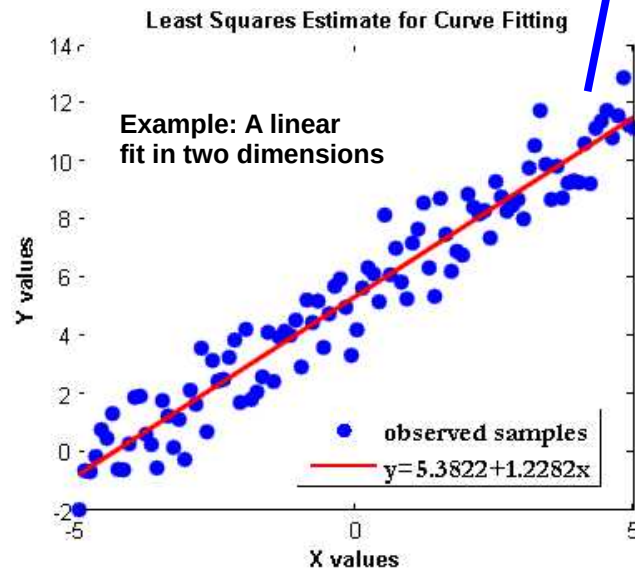
$$\Delta V^0(r) = -k_B T \ln(g^*(r))$$

- \dot{V}^0 also provides a reasonable first potential for IMC

Systematic coarse-graining: Force matching

Main idea: Project the many-body potentials on the function provided by the force-field using a variational principle (least square fit)

$$\chi^2 = \frac{1}{3LN} \sum_{l=1}^L \sum_{i=1}^N |\mathbf{F}_{il}^{\text{ref}} - \mathbf{F}_{il}^p(g_1, \dots, g_M)|^2,$$



$$\begin{cases} a = \frac{(\sum y)(\sum x^2) - (\sum x)(\sum xy)}{n \sum x^2 - (\sum x)^2} \\ b = \frac{n \sum xy - (\sum x)(\sum y)}{n \sum x^2 - (\sum x)^2} \end{cases}$$

<https://mathworld.wolfram.com/LeastSquaresFittingPolynomial.html>

Systematic coarse-graining: Force matching

Main idea: Project the many-body potentials on the function provided by the force-field using a variational principle (least square fit)

L is number of available configurations

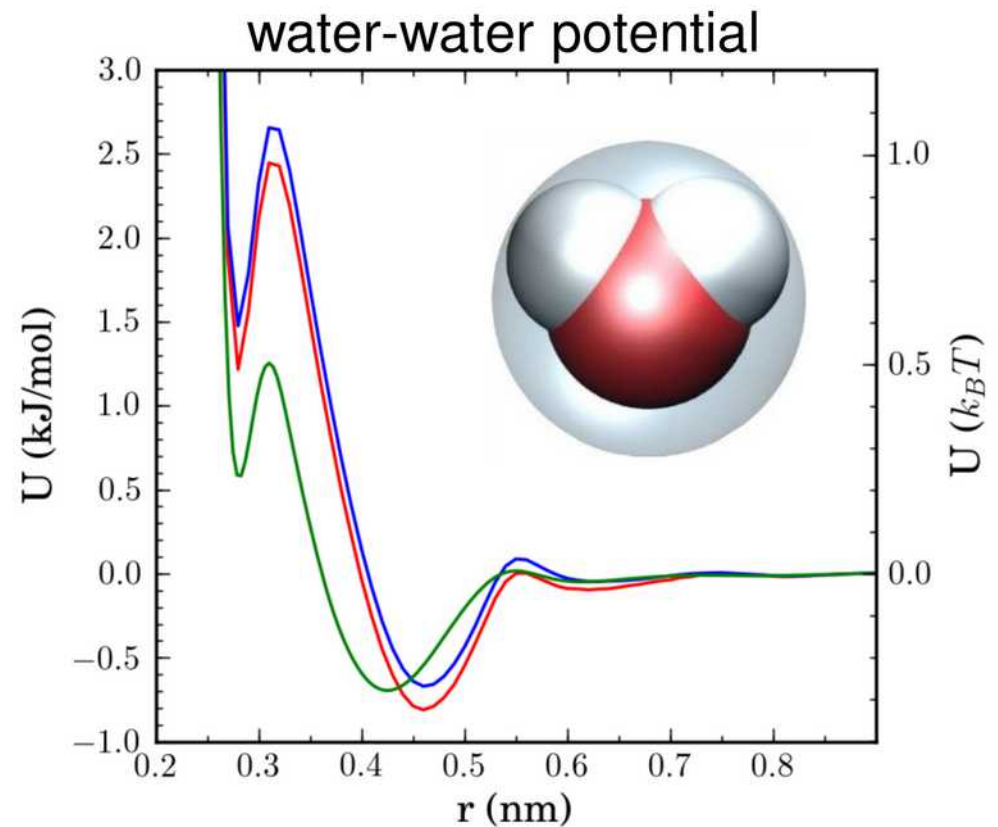
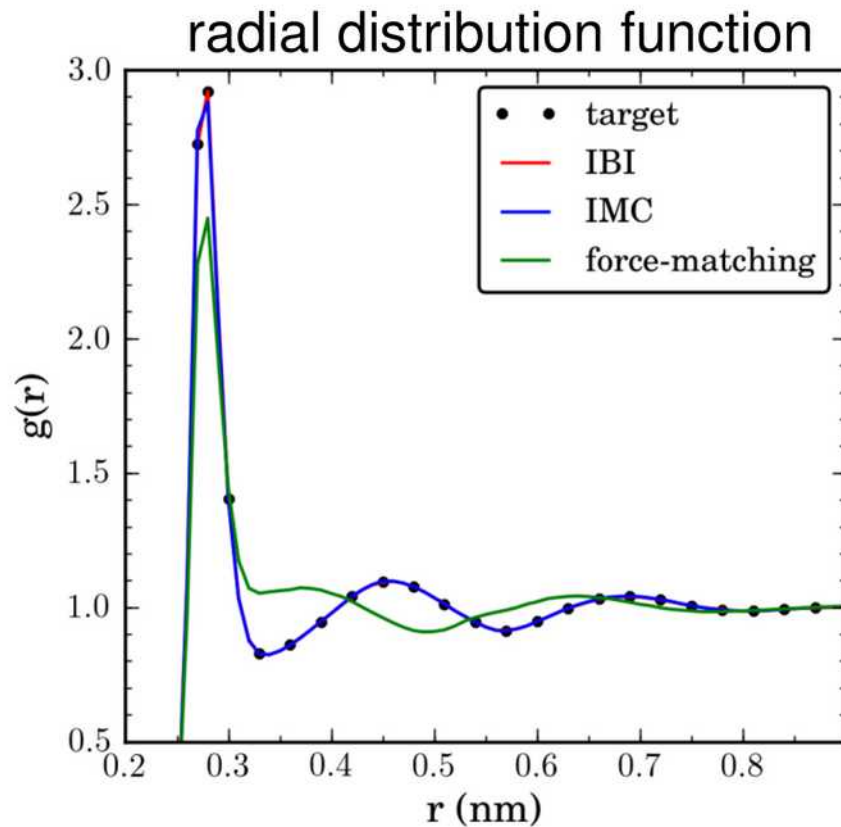
$$\chi^2 = \frac{1}{3LN} \sum_{l=1}^L \sum_{i=1}^N |\mathbf{F}_{il}^{\text{ref}} - \mathbf{F}_{il}^p(\underline{g_1, \dots, g_M})|^2,$$

average resultant reference force (CG)

FF parameters to be fitted

- The Force-field is constructed via a “rerun” over an equilibrated fine-grained trajectory consisting of **L** snapshots.
- Requires knowledge of (mapped) reference forces.
- Pair-wise interactions are introduced explicitly via the rule on how g_1, \dots, g_M determines \mathbf{F}^p

Systematic coarse-graining: Comparison for water molecules



Votca Package, Kremer group, Mainz

Systematic (top-down) coarse-graining

Systematic or top-down coarse-graining:

Pro:

- All one needs is a long equilibrium trajectory of the fine-grained target system to either obtain the RDFs or use it for force-matching.

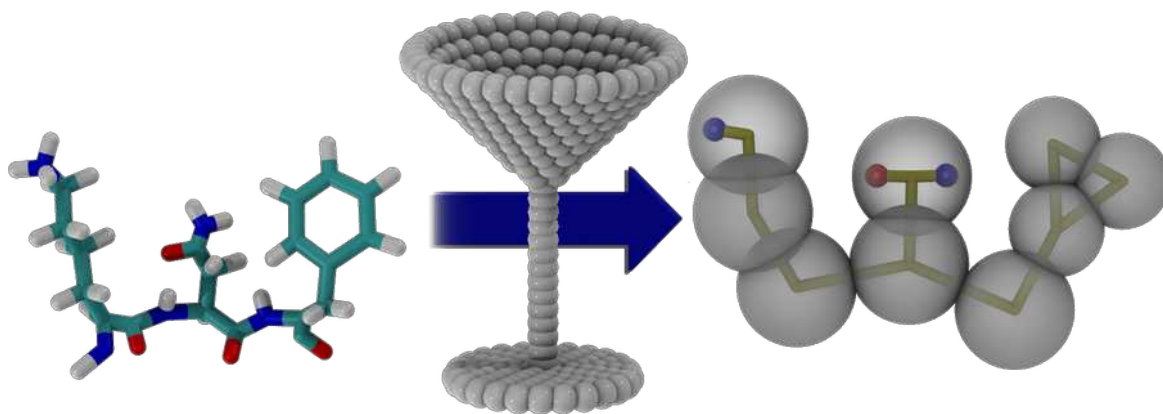
Con:

- The potentials are tuned to describe the system at equilibrium for a particular thermodynamic state point.
- The obtained potentials are 'case' dependent and typically not transverable, i.e., adding additional components may require complete reparametrisation which also implies generating new fine-grained trajectories.

The alternative: Construct highly transferable coarse-grained force-fields from first principles (bottom-up). This is labor intensive and not trivial!

Examples of bottom-up coarse-grained force-field: Martini & Spica

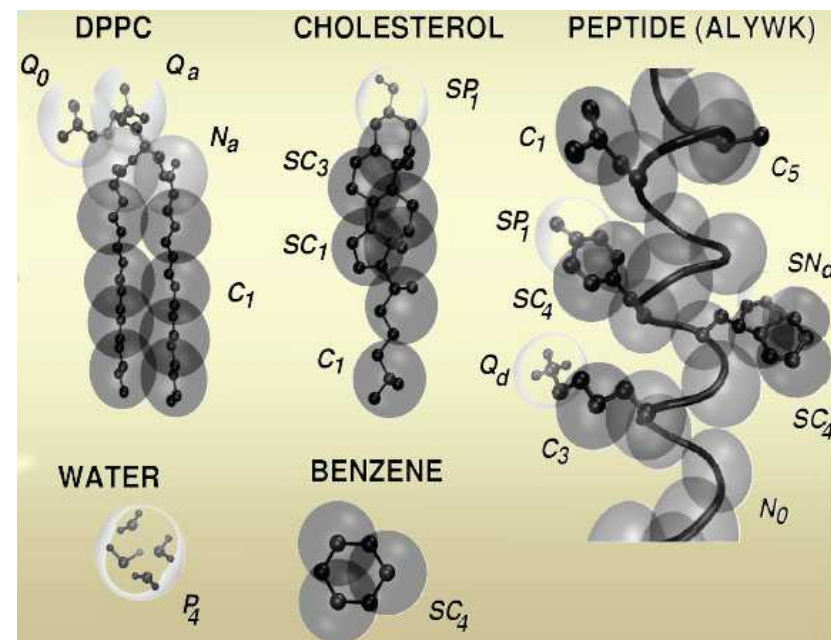
Bottom-up coarse-graining: The Martini model



Standard (!) Lennard-Jones potential:

$$U_{AA} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \alpha \left(\frac{\sigma}{r} \right)^6 \right]$$

GROMACS
fast, flexible & free



- The 'superatom' approach: several atoms modeled as a single 'atom'.

The gain: $\Delta t \times 10$ & $N/4$ & Diffusion $\times 4 \Rightarrow 160x$ speed up!

SJ Marrink, HJ Risselada, ..., AE Mark, J. Phys. Chem. B, 7812-7824, 2007


Bottom-up coarse-graining: Martini model

Main idea: Construct universally compatible interaction types for functional chemical groups commonly found within biomolecules. Then build new molecules like building with “lego” blocks.

Chose ϵ and σ such that thermodynamic properties are reproduced

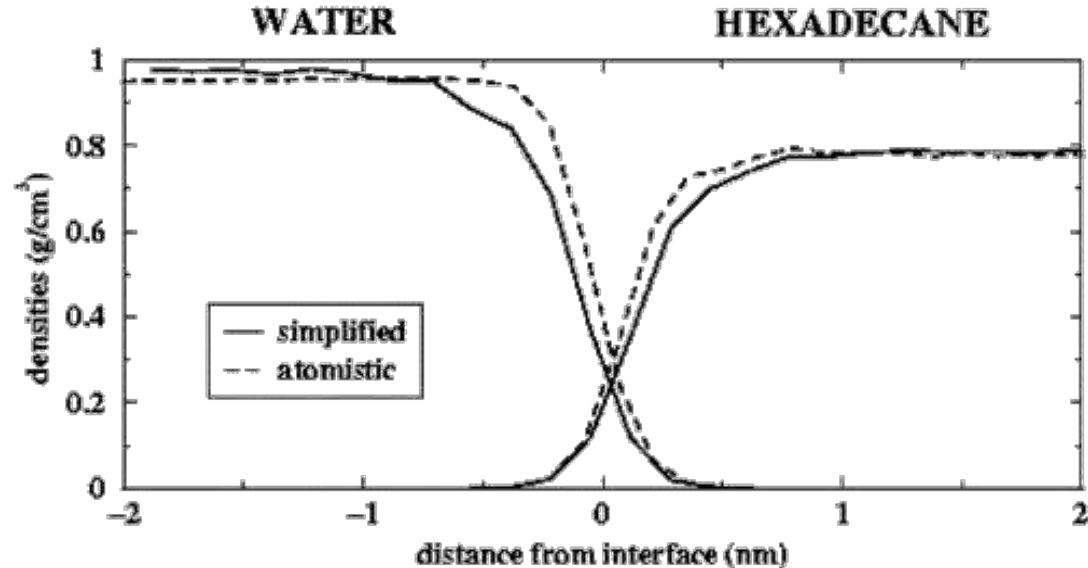
TABLE 2: Properties of Water and Alkanes with the CG Model Compared to Experimental Values^a

system	CG model	density, ^b g cm ⁻³	compressibility, ^c 10 ⁻⁵ bar ⁻¹	diffusion, ^d 10 ⁻⁵ cm ² s ⁻¹
water	P	0.99 (0.99)	6 (4.5)	2.0 (2.3)
butane	C	0.68 (0.58)	28 (> 17)	1.9 (> 5)
hexane	C-C	0.58 (0.66)	14 (17)	0.7 (4)
octane	C-C	0.77 (0.70)	14 (13)	0.6 (2)
decane	C-C-C	0.67 (0.73)	12 (11)	0.35 (1)
dodecane	C-C-C	0.80 (0.75)	12 (10)	0.3 (-)
tetradecane	C-C-C-C	0.71 (0.76)	12 (9)	0.25 (-)
hexadecane	C-C-C-C	0.81 (0.77)	12 (9)	0.2 (-)
octadecane	C-C-C-C-C	0.74 (0.78)	11 (-)	0.2 (0.3)
eicosane	C-C-C-C-C	0.82 (0.79)	11 (-)	0.15 (-)


$$U_{AA} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \alpha \left(\frac{\sigma}{r} \right)^6 \right]$$

^a Properties at 300 K, unless specified. Experimental properties are given in parentheses. ^b Experimental densities at 293 K.²⁰ ^c Experimental isothermal compressibilities from ref 20. The values from simulations are computed from the volume fluctuations in an NPT ensemble. ^d Diffusion rates were obtained from the slope of the mean squared displacement (MSD) curve in the long time limit. Experimental values extrapolated from temperature-dependent data.²¹

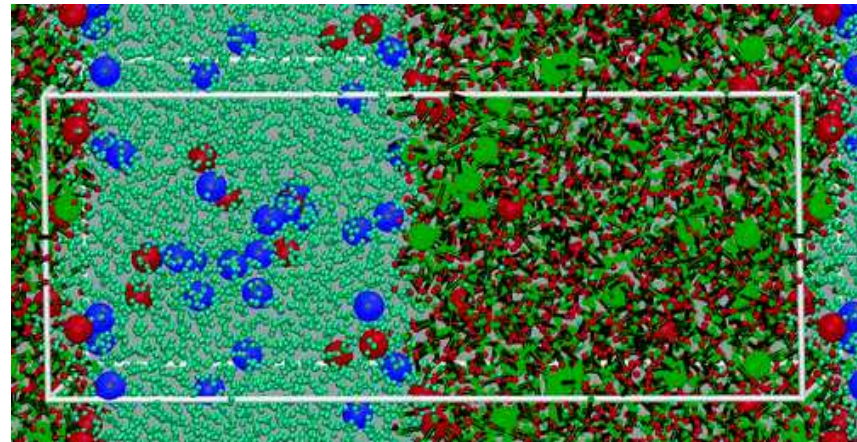
Bottom-up coarse-graining: Martini model



Lorentz-Berthelot rules:

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2}$$

$$\epsilon_{ij} = \sqrt{\epsilon_{ii}\epsilon_{jj}}$$



Martini force-field does not reproduce surface tensions because its usage of a LJ12-6 potential!

Bottom-up coarse-graining: Martini model

Example: Note that sigma is 0.47, mass is 72 u, and only ϵ differs between the 5 different interactions types

$$U_{AA} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \alpha \left(\frac{\sigma}{r} \right)^6 \right]$$

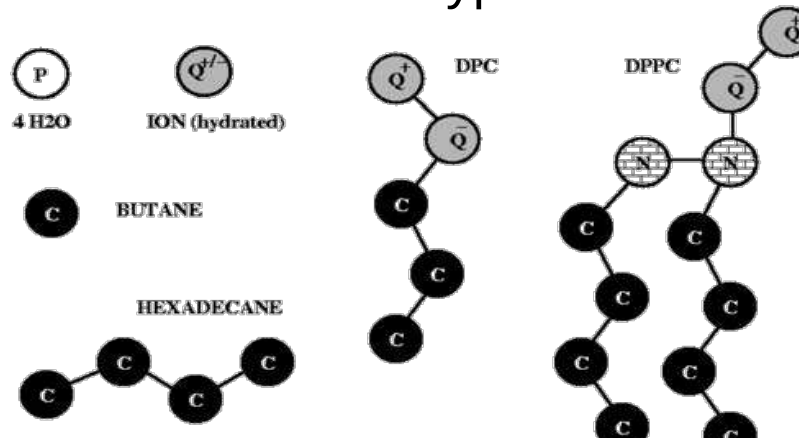


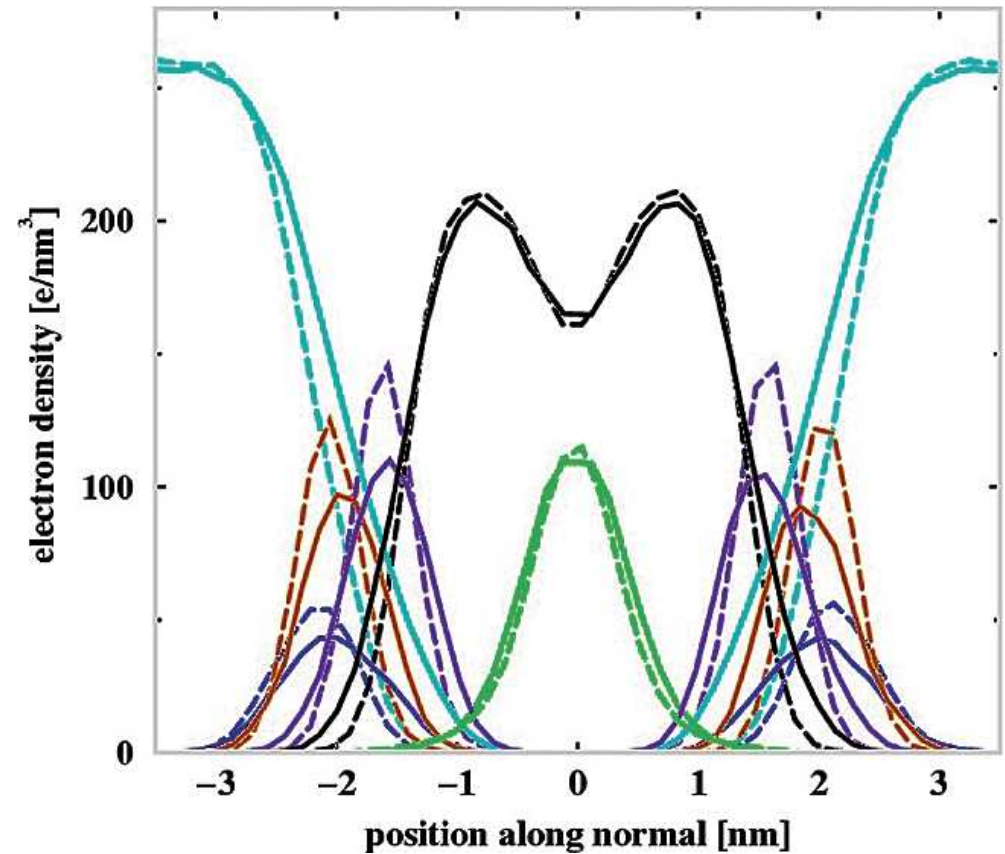
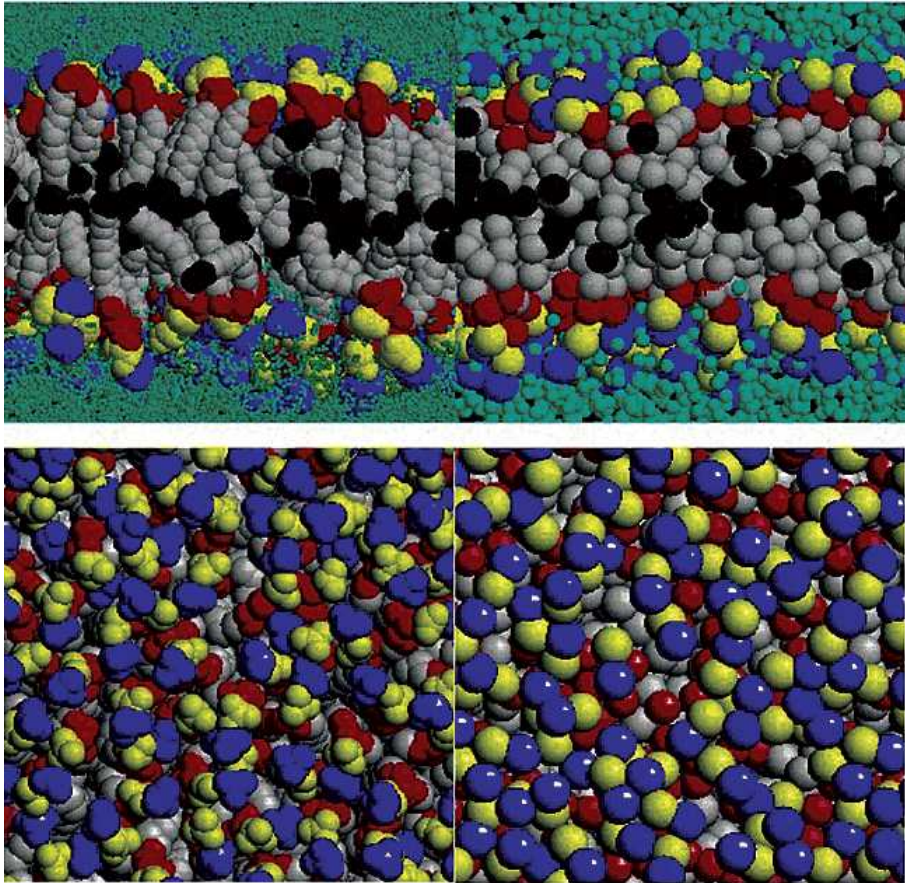
TABLE 1: Interaction Matrix^a

group	subtype	P	N				C	Q			
			0	d	a	da		0	d	a	da
P		I	IV	III	III	II	V	I	I	I	I
N	0	IV	III	III	III	III	III	III	III	III	III
	d	III	III	II	II	II	IV	III	III	II	II
	a	III	III	II	II	II	IV	III	II	III	II
	da	II	III	II	II	I	V	III	II	II	I
C		V	III	IV	IV	V	III	V	V	V	V
Q	0	I	III	III	III	III	V	III	III	III	II
	d	I	III	III	II	II	V	III	III	II	I
	a	I	III	II	III	II	V	III	II	III	I
	da	I	III	II	II	I	V	II	I	I	I

^a Level of interaction I (attractive), II (semi-attractive), III (intermediate), IV (semi-repulsive) or V (repulsive). Four different groups are considered: polar (P), nonpolar (N), apolar (C), and charged (Q). Both groups N and Q have four subtypes: 0 for no hydrogen bonding capabilities present, d for groups acting as hydrogen bond donor, a for groups acting as hydrogen bond acceptor, and da for groups with both donor and acceptor options.

The goal is to minimize the number of interaction types required to describe all possible molecules!

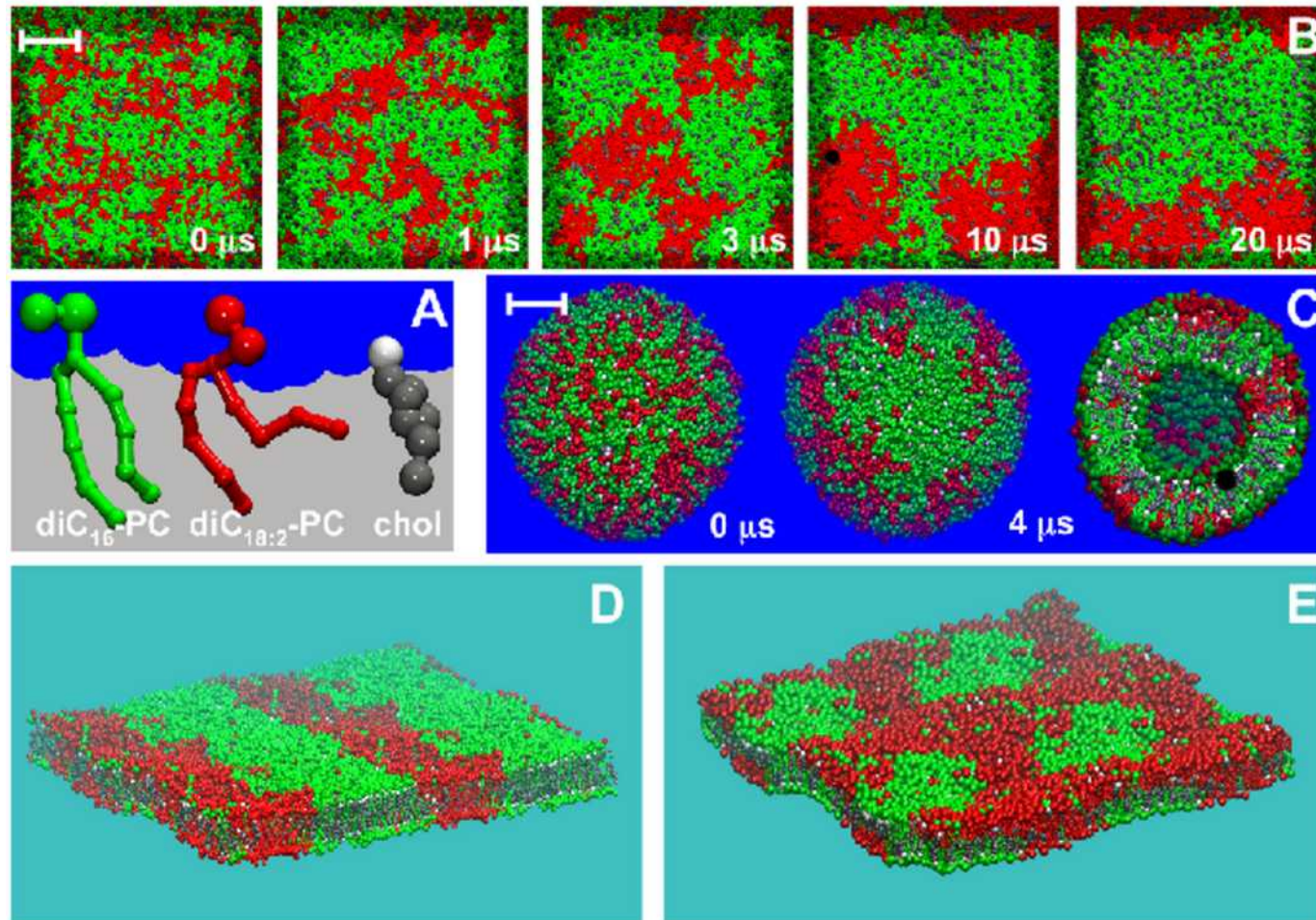
Bottom-up coarse-graining: Martini model



SJ Marrink, *HJ Risselada*,..., AE Mark, J. Phys. Chem. B, 7812-7824, 2007

Bottom-up coarse-graining: Martini model

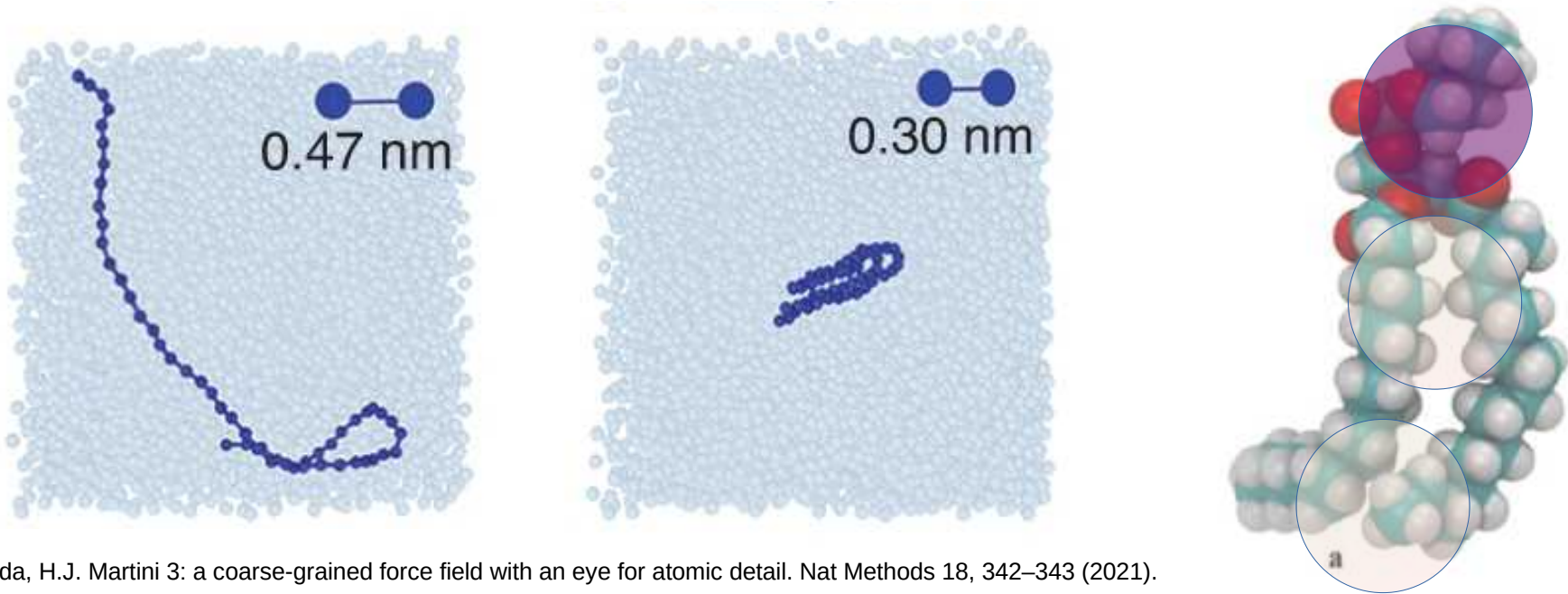
Simulation of the liquid ordered/disorder phase separation in ternary mixtures



HJ Risselada, SJ Marrink, PNAS, 17367-17372, 2008

Bottom-up coarse-graining: A general challenge

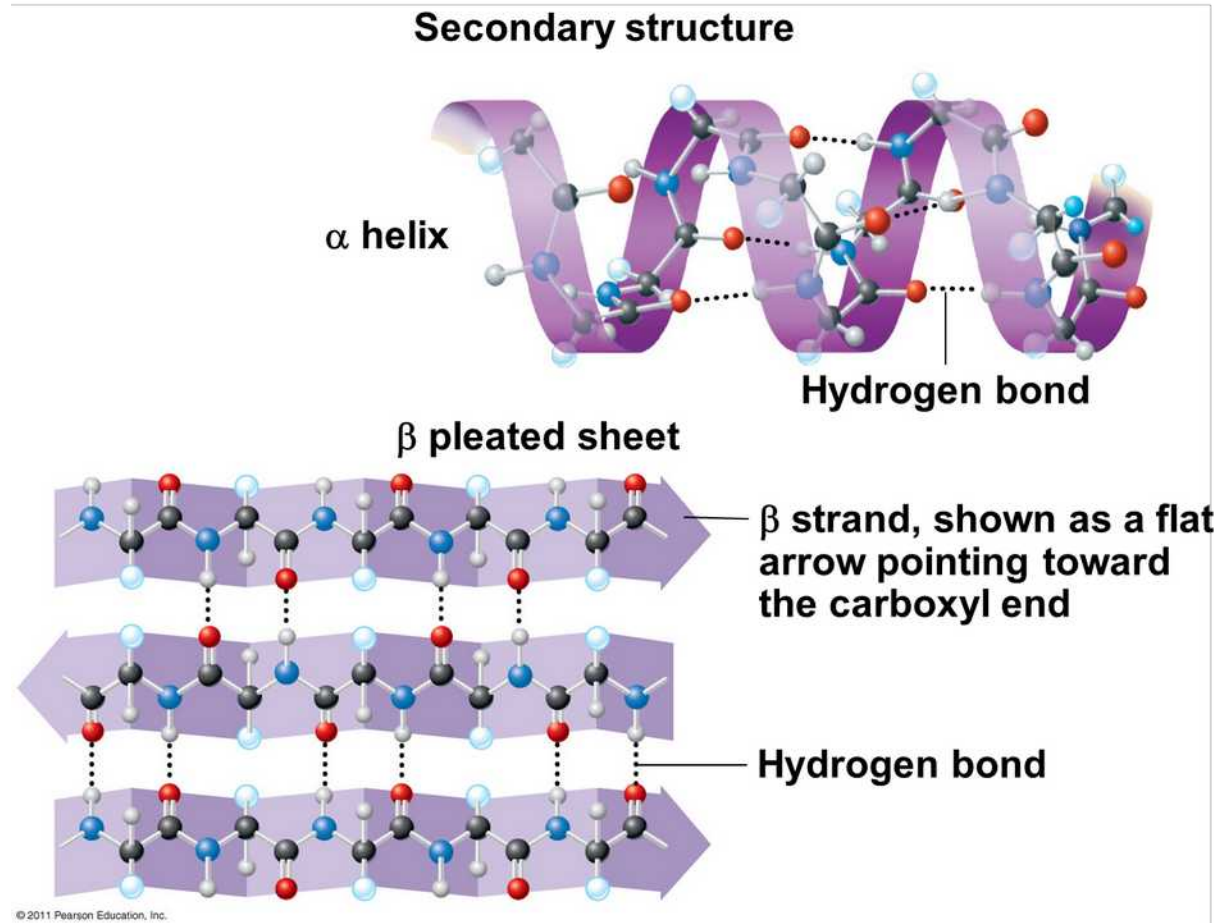
Bonded and non-bonded interactions are not independent!



Risselada, H.J. Martini 3: a coarse-grained force field with an eye for atomic detail. Nat Methods 18, 342–343 (2021).

- The bond length between CG beads is not uniquely defined.
- Bonded and non-bonded interactions must be optimized/parametrized simultaneously!
- Labor intensive & independent people work on dependent parameters.

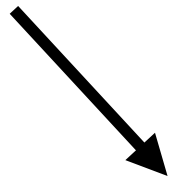
Bottom-up coarse-graining: A general challenge



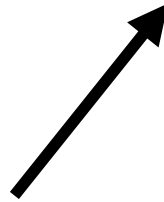
- Irrelevant degrees of freedom are not always irrelevant!

Bottom-up coarse-graining: A general challenge

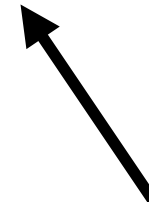
Reproduced!



$$\Delta G = \Delta H - T \Delta S$$



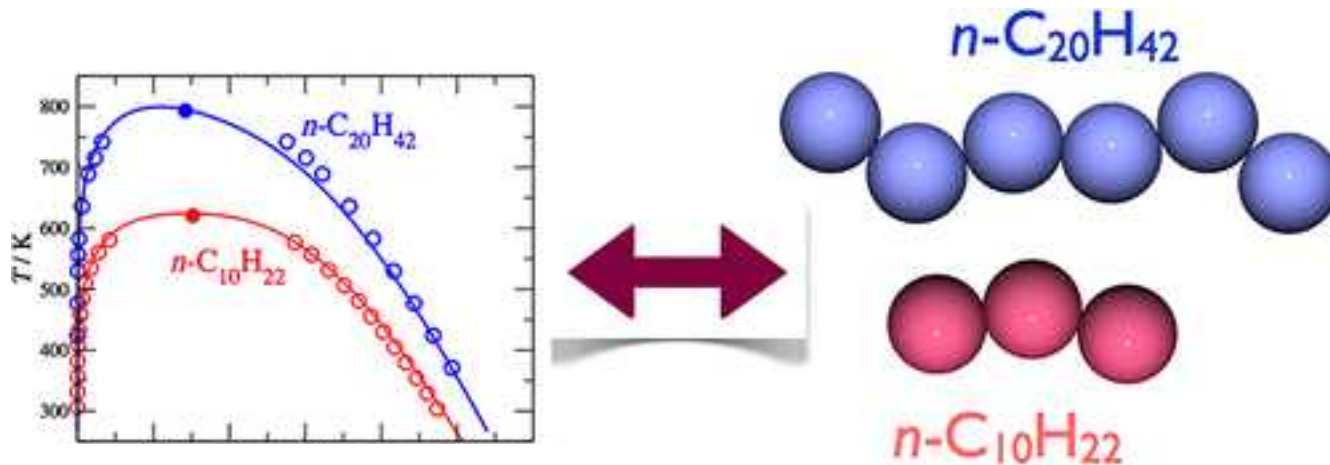
Compensated!



Not reproduced!

The prediction of phase behavior in bottom-up force-fields like Martini is only “accurate” when the phase transition temperature lies close to the temperature of parametrization (room temperature).

Top-down coarse-graining over a large temperature range: the statistical associating fluid theory (SAFT-gamma)



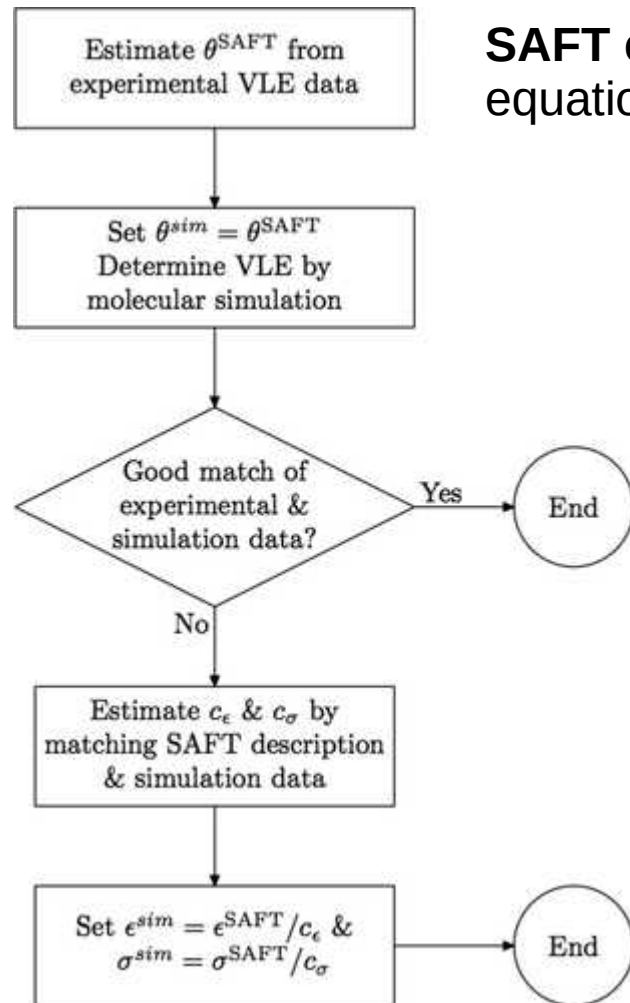
$$u^{\text{Mie}}(r) = C\epsilon \left[\left(\frac{\sigma}{r} \right)^{\lambda_r} - \left(\frac{\sigma}{r} \right)^{\lambda_a} \right] \quad C = \frac{\lambda_r}{\lambda_r - \lambda_a} \left(\frac{\lambda_r}{\lambda_a} \right)^{\lambda_a / (\lambda_r - \lambda_a)}$$

Avendano, C., Lafitte, T., Galindo, A., Adjiman, C. S., Jackson, G., & Müller, E. A. (2011). SAFT-γ force field for the simulation of molecular fluids. 1. A single-site coarse grained model of carbon dioxide. The Journal of Physical Chemistry B, 115(38), 11154-11169.

Avendaño, C., Lafitte, T., Adjiman, C. S., Galindo, A., Müller, E. A., & Jackson, G. (2013). SAFT-γ force field for the simulation of molecular fluids: 2. Coarse-grained models of greenhouse gases, refrigerants, and long alkanes. The Journal of Physical Chemistry B, 117(9), 2717-2733

- Use the vapor (saturation) pressure and saturated-liquid density data over a wide range of temperatures as target properties

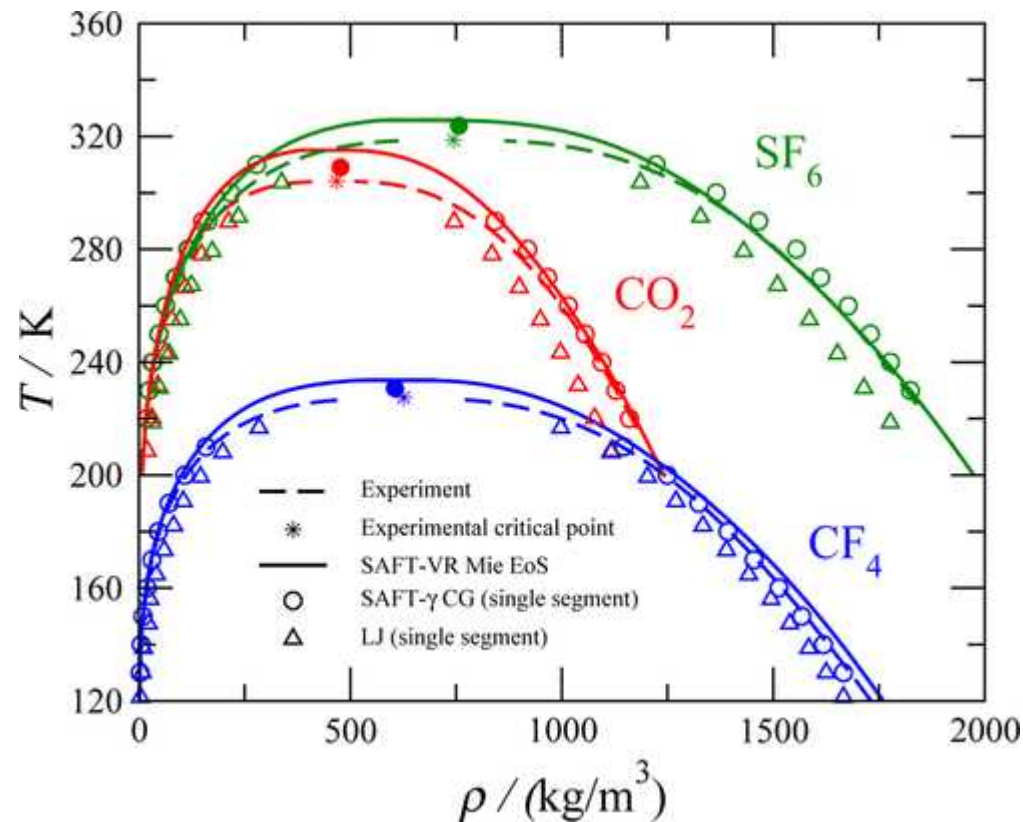
Top-down coarse-graining: SAFT Force-Field



SAFT equations: Analytical relationships between the equations of state (g(r)) and the pair-wise interaction parameters.

$$\begin{aligned}
 & \min_{\sigma, \epsilon, \lambda_r, \lambda_a, m_s} F_{\text{obj,exp}}(\sigma, \epsilon, \lambda_r, \lambda_a, m_s) \\
 &= \min_{\sigma, \epsilon, \lambda_r, \lambda_a, m_s} \left\{ \sum_{i=1}^{N_p} \left(\frac{P_v^{\text{SAFT}}(T_i; \sigma, \epsilon, \lambda_r, \lambda_a, m_s) - P_v^{\text{exp}}(T_i)}{P_v^{\text{exp}}(T_i)} \right)^2 \right. \\
 & \quad \left. + \sum_{j=1}^{N_\rho} \left(\frac{\rho_1^{\text{SAFT}}(T_j; \sigma, \epsilon, \lambda_r, \lambda_a, m_s) - \rho_1^{\text{exp}}(T_j)}{\rho_1^{\text{exp}}(T_j)} \right)^2 \right\} \quad (3)
 \end{aligned}$$

Top-down coarse-graining: SAFT Force-Field



Avendaño, C., Lafitte, T., Adjiman, C. S., Galindo, A., Müller, E. A., & Jackson, G. (2013). SAFT- γ force field for the simulation of molecular fluids: 2. Coarse-grained models of greenhouse gases, refrigerants, and long alkanes. *The Journal of Physical Chemistry B*, 117(9), 2717-2733

Done.....

