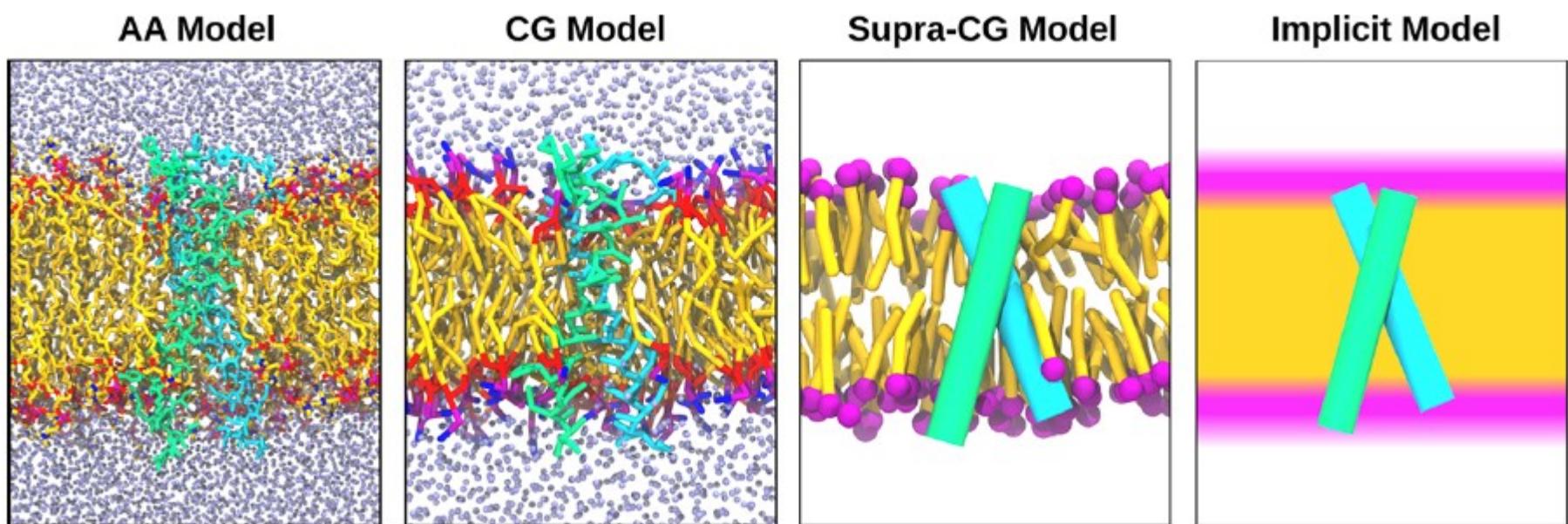
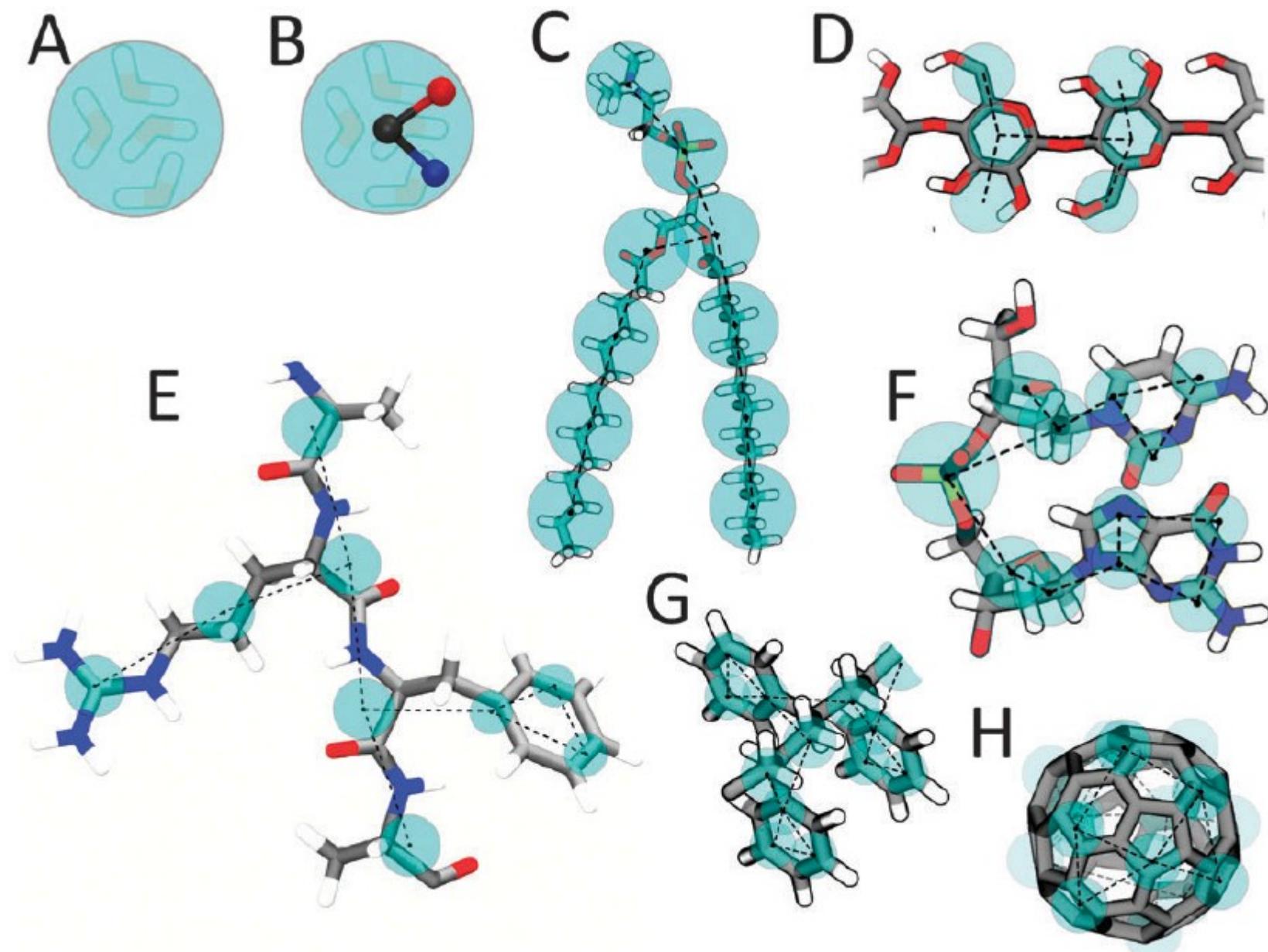


Coarse-graining



Martini coarse-grained mapping



All-atom vs. MARTINI coarse-graining

All atom MD:

- Computationally costly
- Sometimes too much detail is not needed
- 1 particle → 1 atom
- Size: (1-10-100 nm)³
- Time: 10⁻⁷-10⁻⁵-10⁻³s
- DT=1 or 2 fs (to capture fastest degrees of freedom)

Coarse-grain Martini MD:

- Computationally efficient
- Removal of atomic detail
- 1 particle → 3-4 atoms
- Size: (1-10-100 nm)³
- Time: 10⁻⁷-10⁻⁵-10⁻³s
- DT=20-30 fs



Martini interactions

Non-bonded interactions

- Lennard-Jones potential:
strength:

ϵ : 2.0 kJ/mol → polar – apolar groups

...

ϵ : 5.6 kJ/mol → strongly polar groups

Effective (bead) size:

$\sigma \sim 0.47$ nm

- Electrostatic interactions:

Some bead types are charged

Screened ($\epsilon_{\text{rel}} = 15$)

Bonded interactions

- bonds, angles, dihedrals
- parameters obtained to fit either original molecular structural data or atomistic simulations

Validation:

Comparison against experimental or all-atom data:

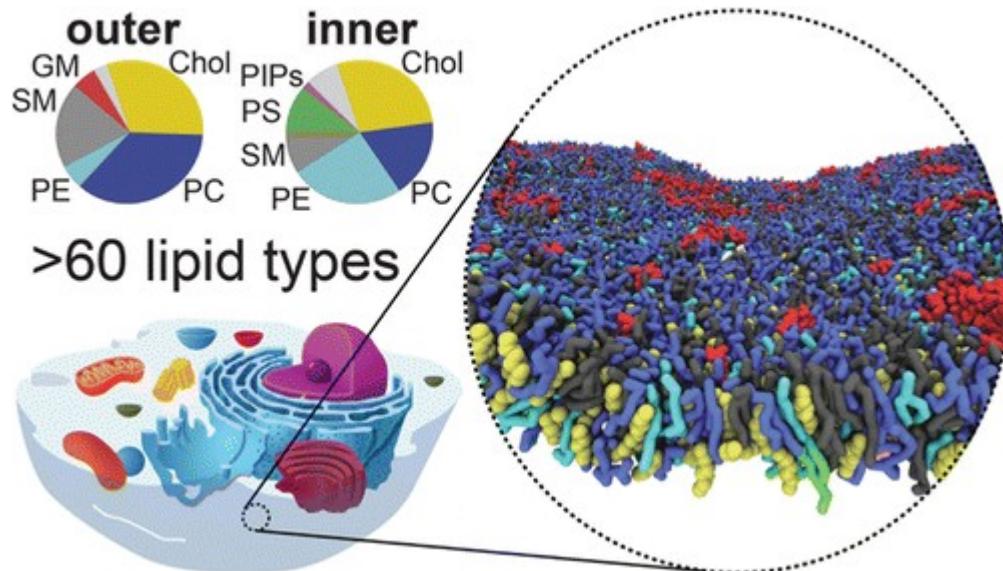
- partition of amino-acid side chain analogues (SCAs) in membranes (error $\sim 1-2 k_B T$)

- dimerization of SCAs in solvents of different polarity (error $\sim 1 k_B T$)

- PMFs contrasted to all atom data

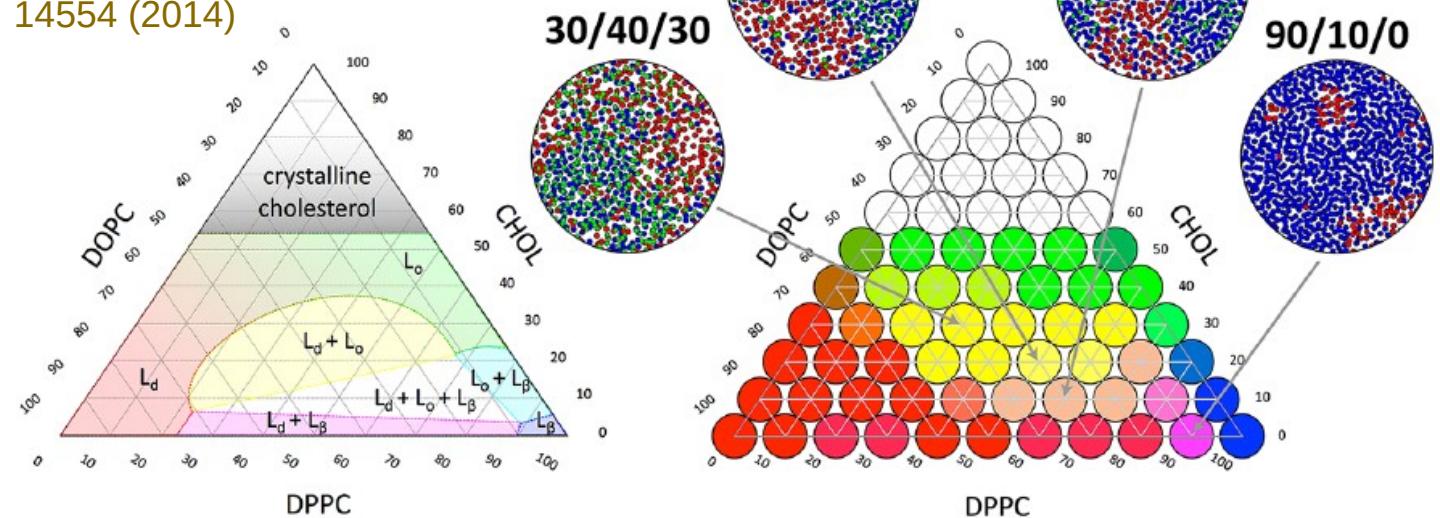
Applications: complex bilayers && systematic variation of lipid composition

Plasma membrane:



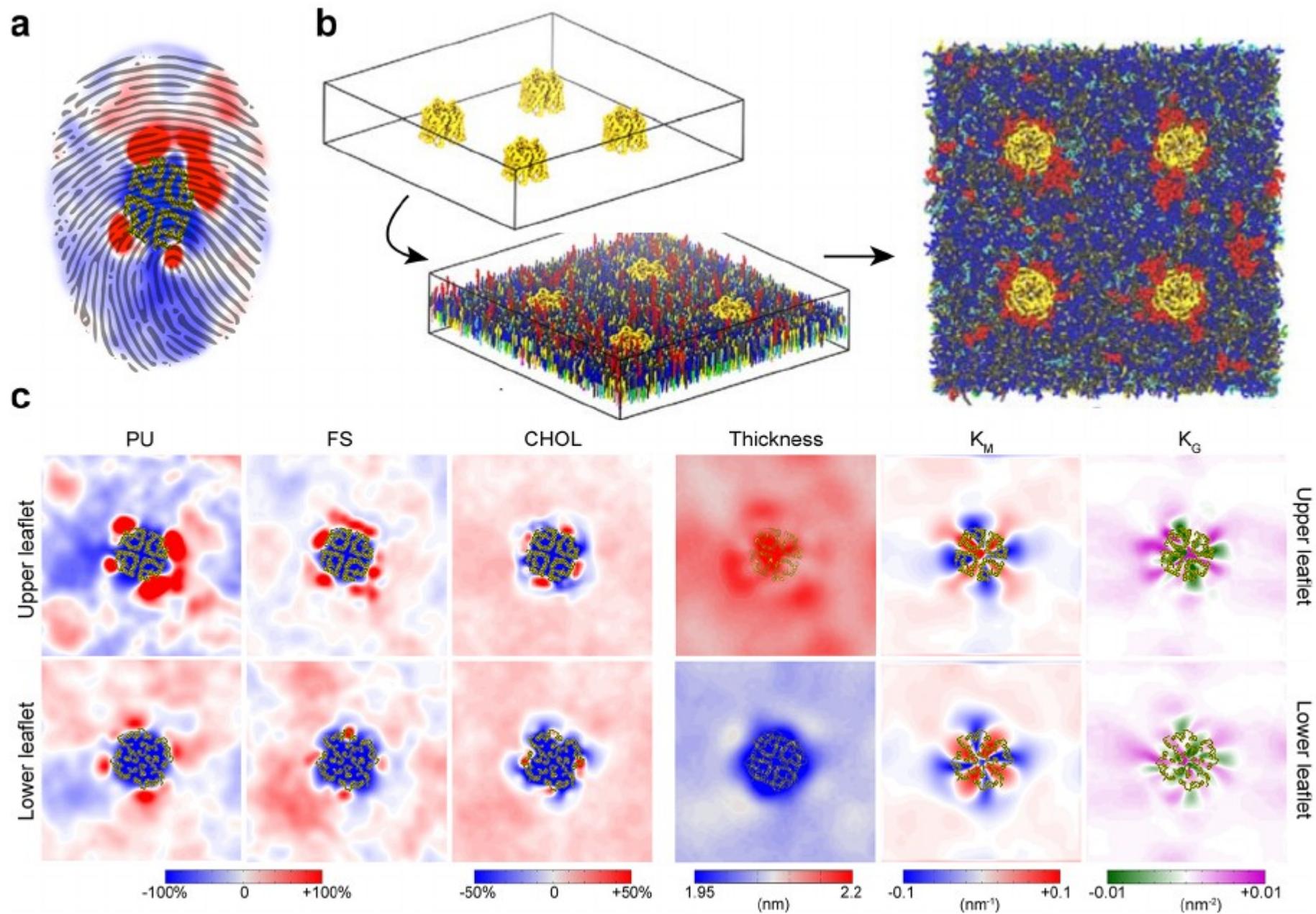
From: Ingólfsson et al. JACS 136: 14554 (2014)

Phase-diagrams of ternary lipid mixtures

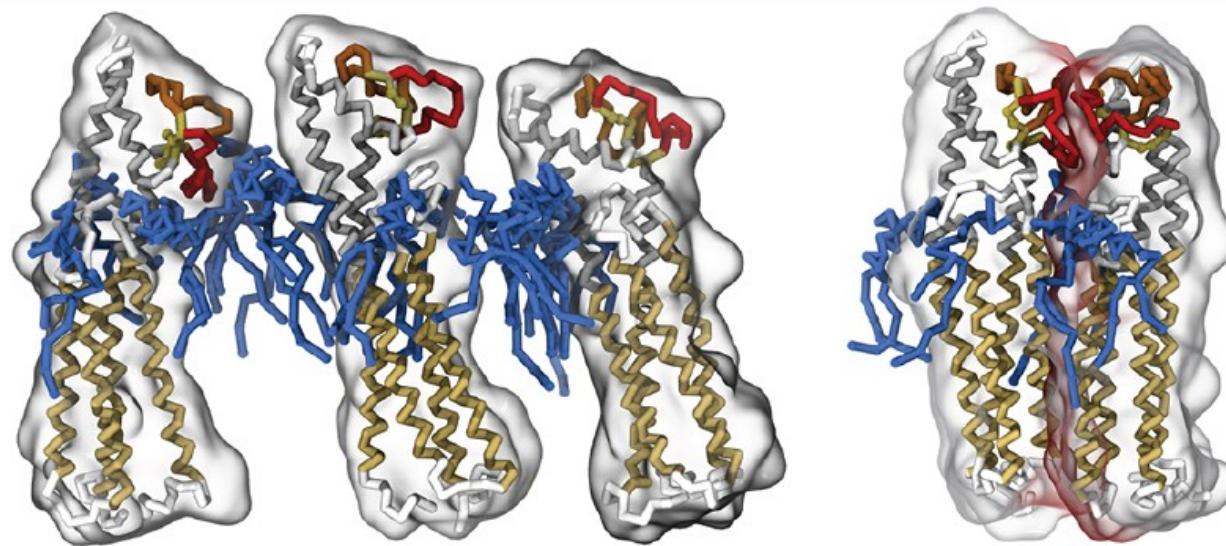
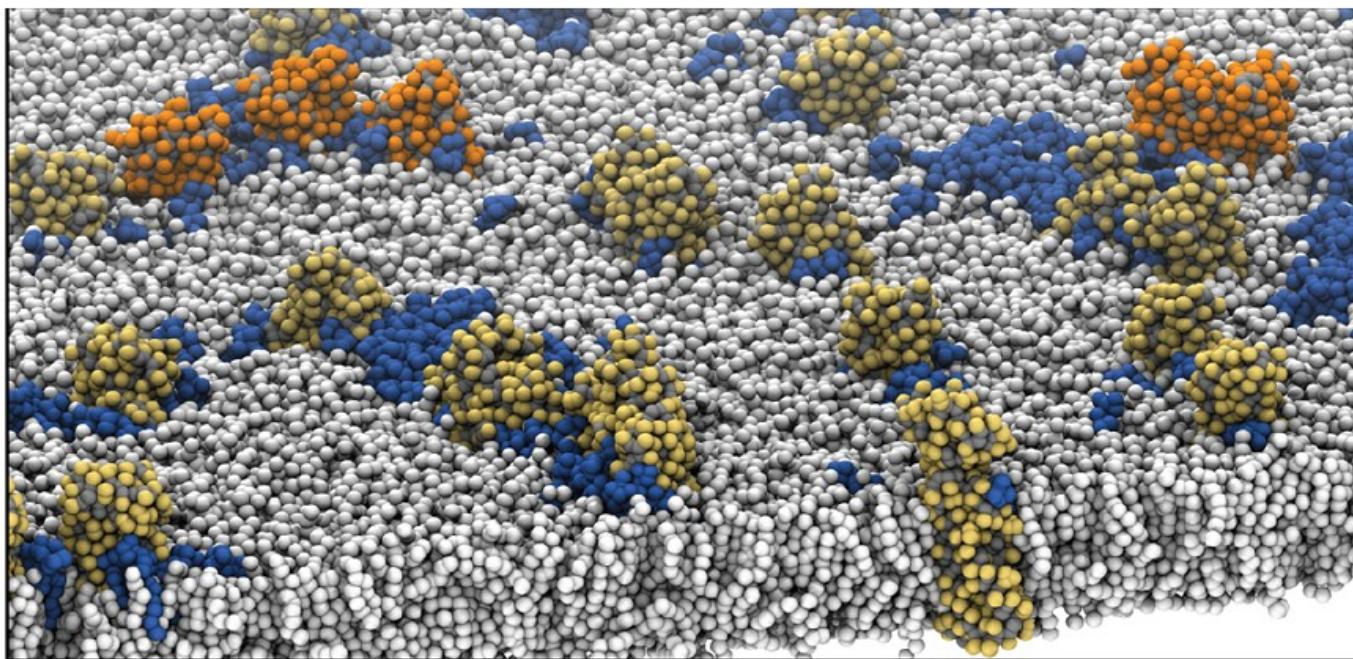


From: Carpenter et al. JCTC. 14:6050–6062 (2018)

Applications: Lipid-protein interactions

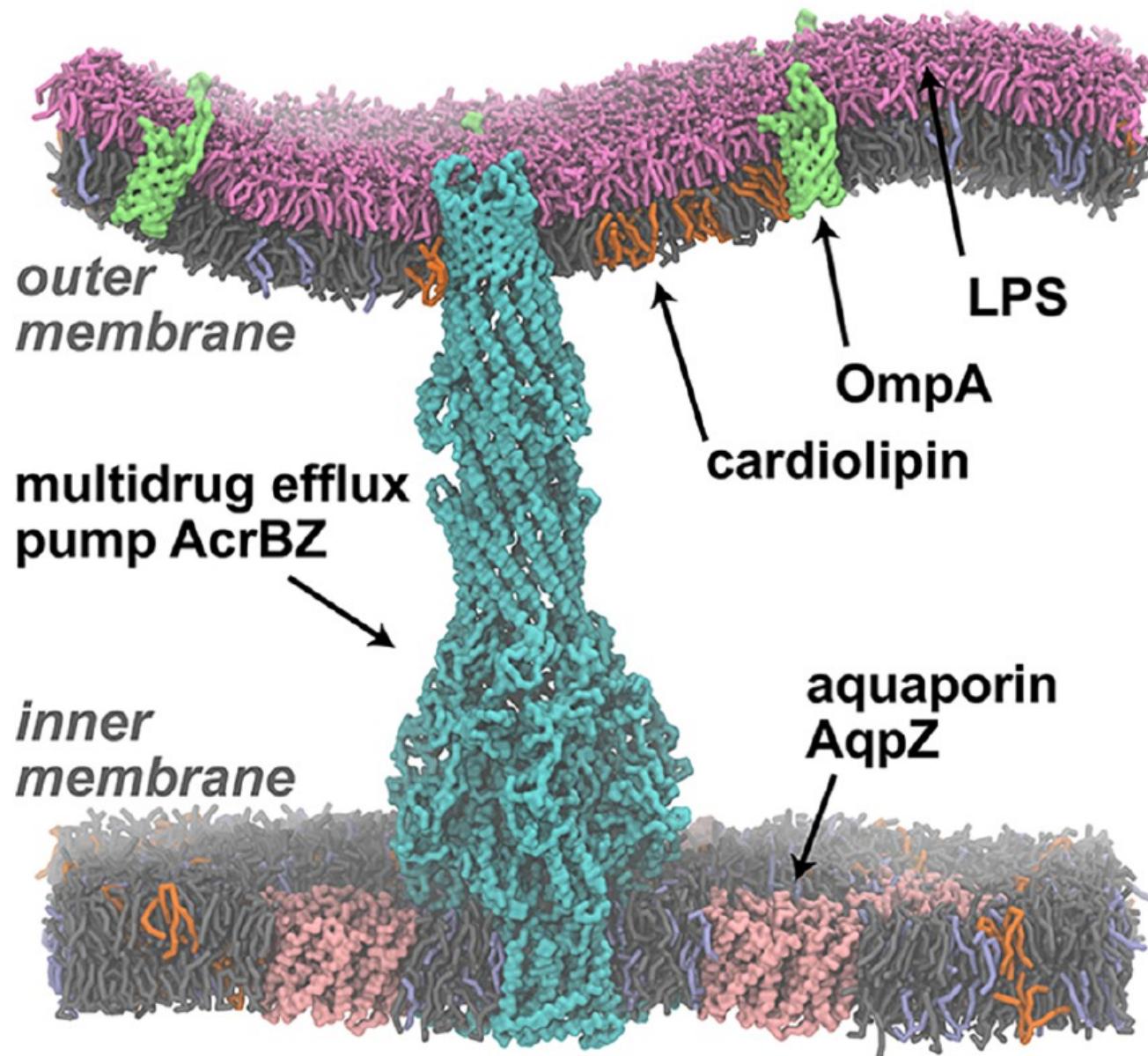


Applications: protein-protein oligomerization

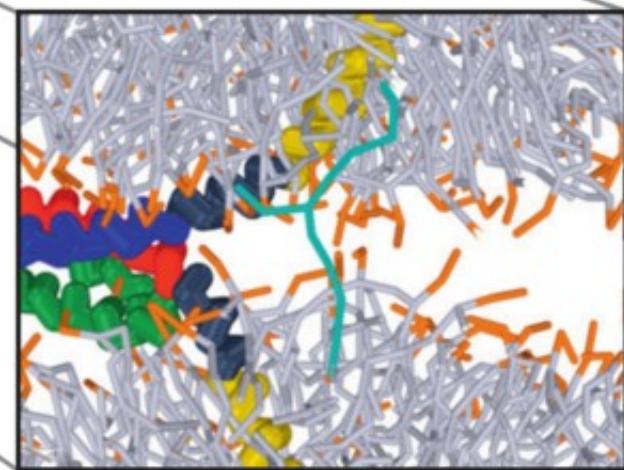
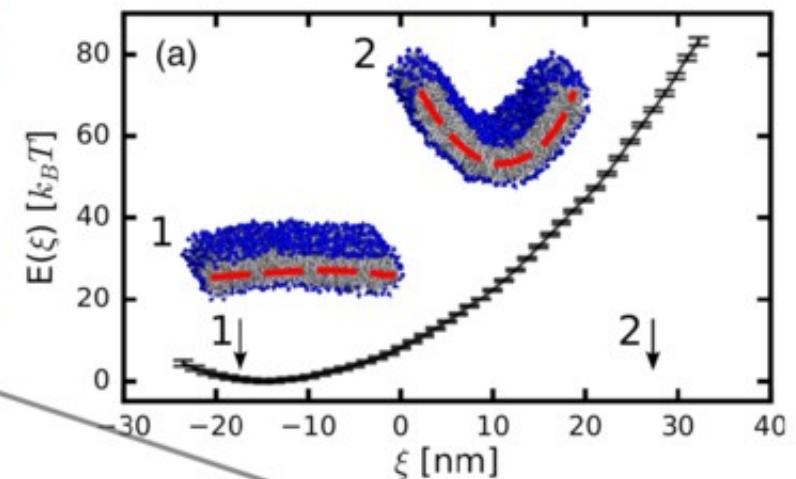
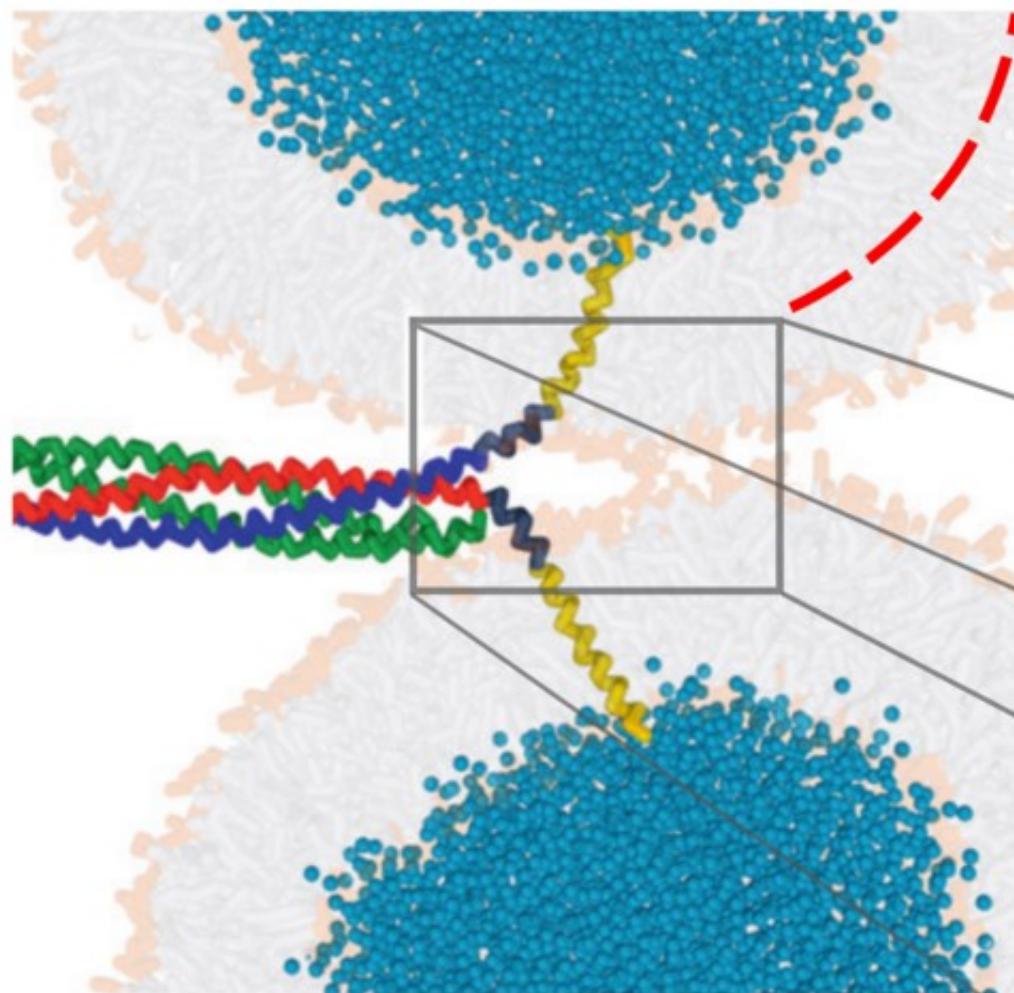


From: Schmidt, T et al. Biophys. J. 2016, 110, 2463–2474.

Applications: simulation of bacterial membranes



Applications: vesicle fusion

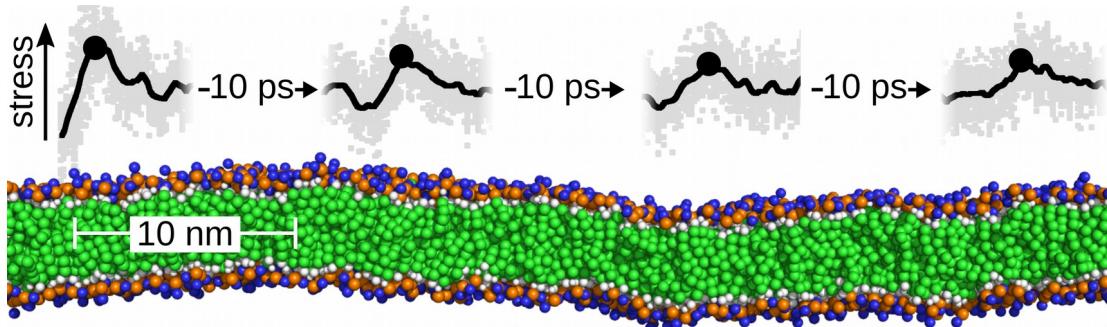


Applications: biological lipid bilayers stress propagation through and mechanical indentation

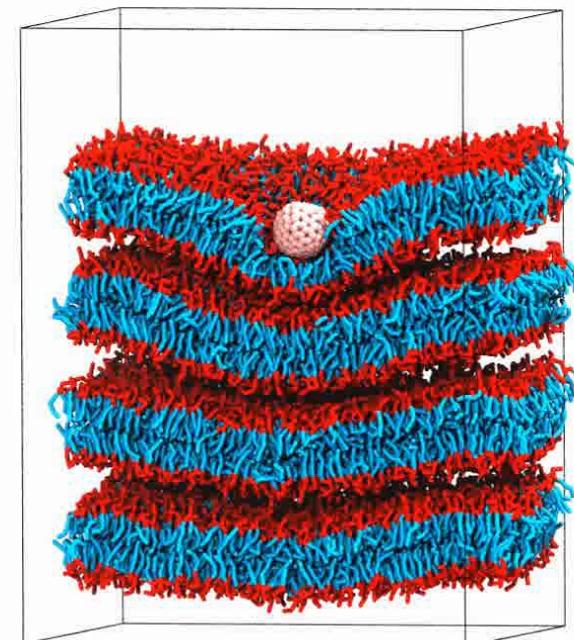


Stress propagation through lipid bilayers

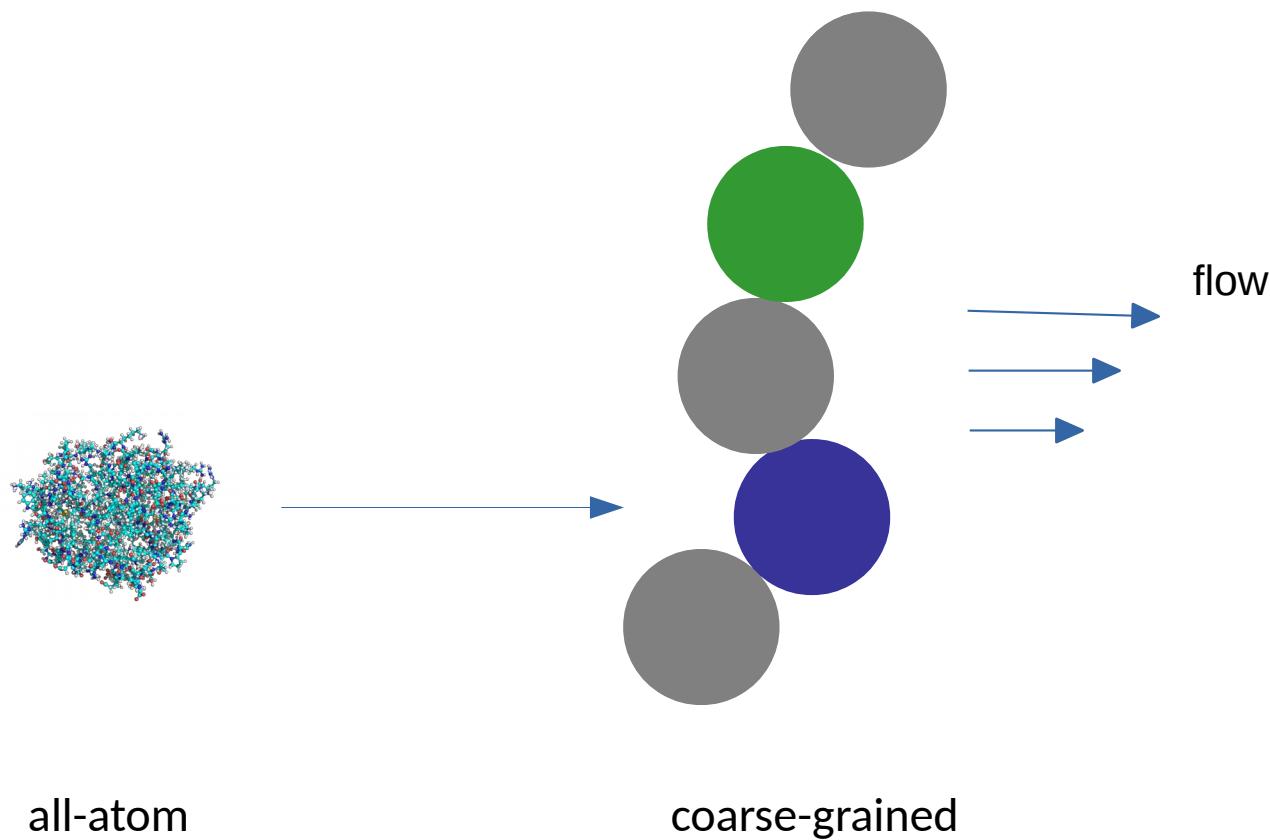
CA-S, Brunkent, Gräter. JACS. 2017



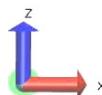
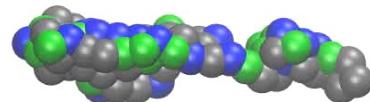
Indentation of
stacked lipid bilayers
Franz, CA-S, Daday,
Miletic, Gräter. JPCB. 2018



Ultra coarse-graining: Response of multi-domain protein to blood flow



Ultra coarse-graining: Response of multi-domain protein to blood flow



Challenges and limitations

- Force-field:
derivation of interaction
parameters
- Water polarizability
- Protein conformational changes
- Molecular processes
(e.g. water or ion permeation)