

Membrane modelling and protein interactions



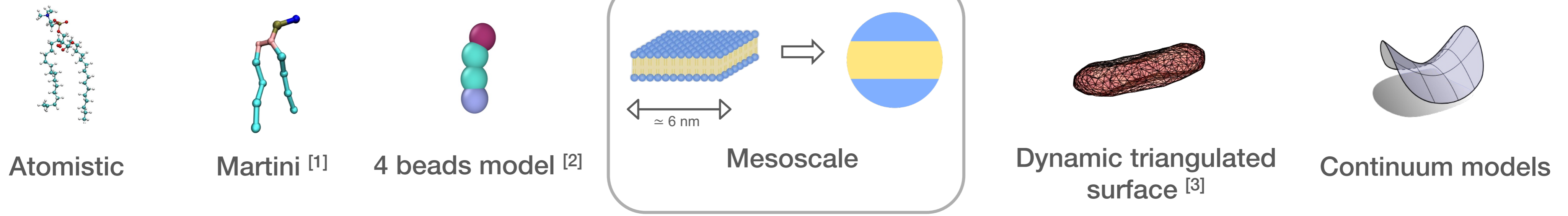
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Spatial and temporal scales

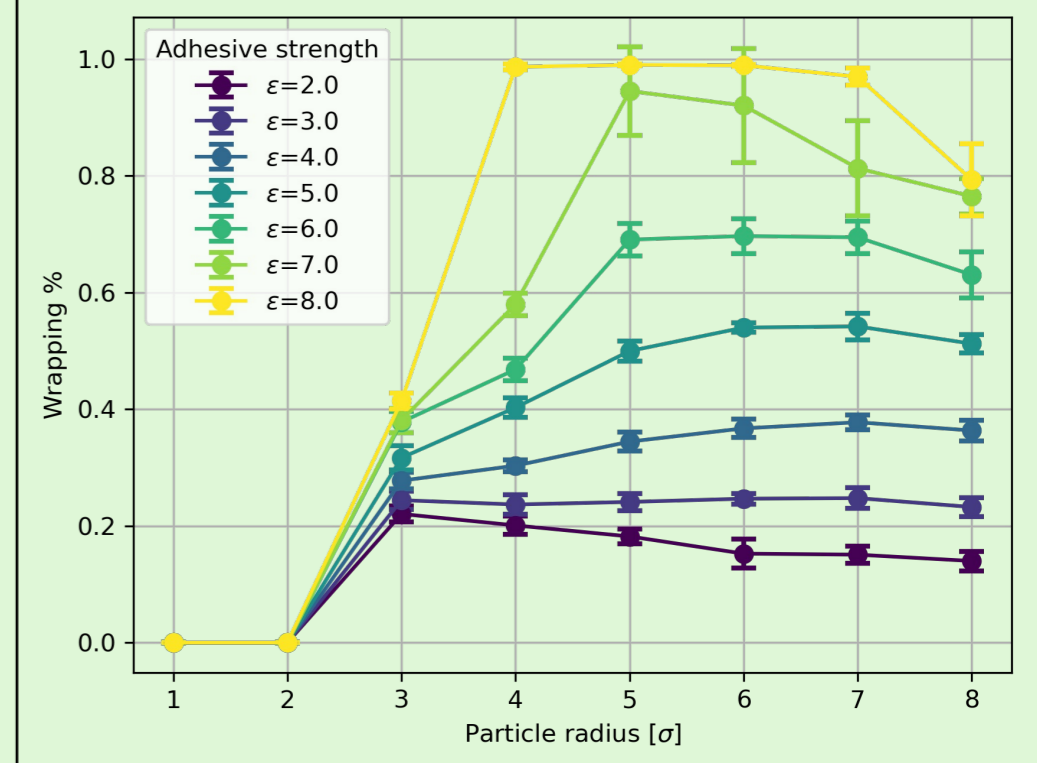
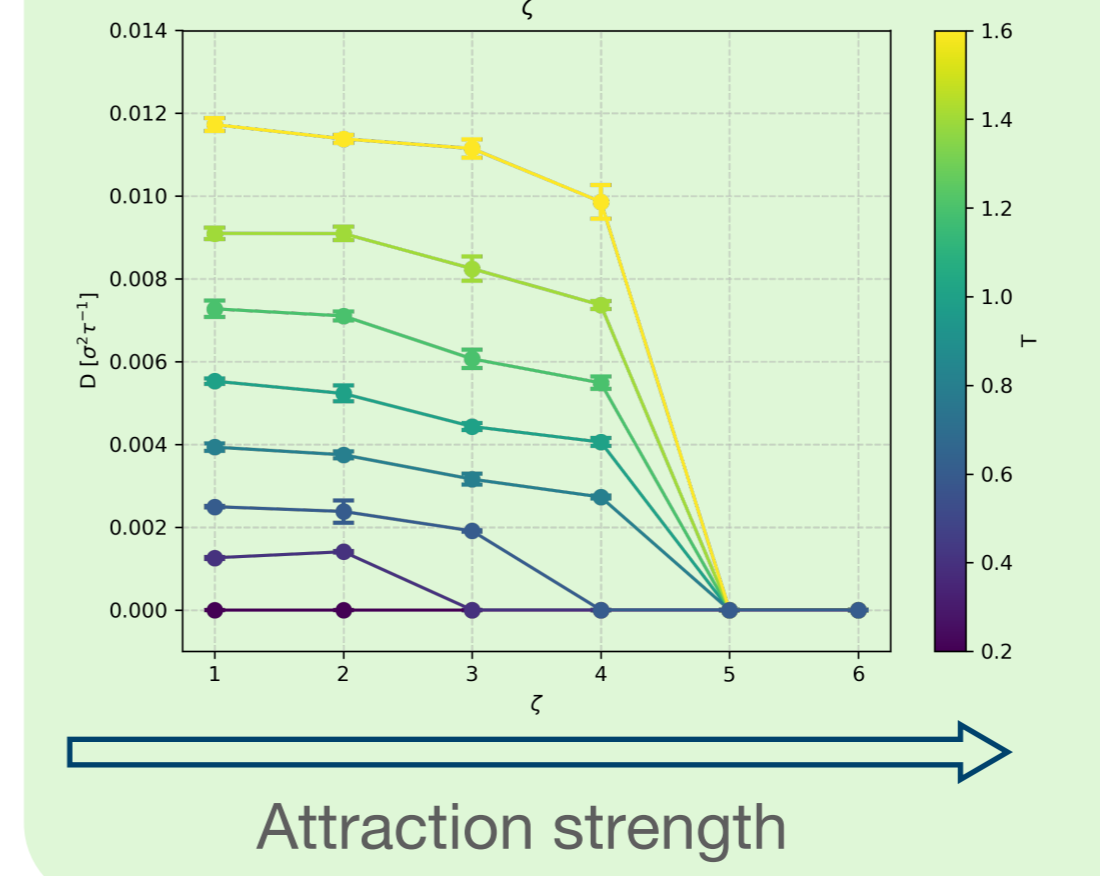
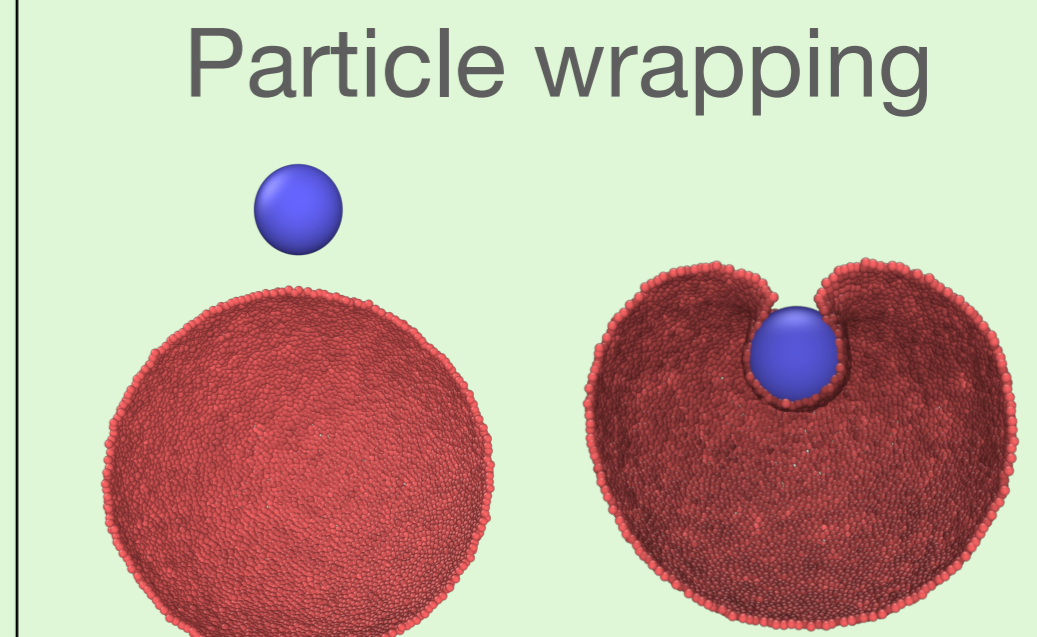
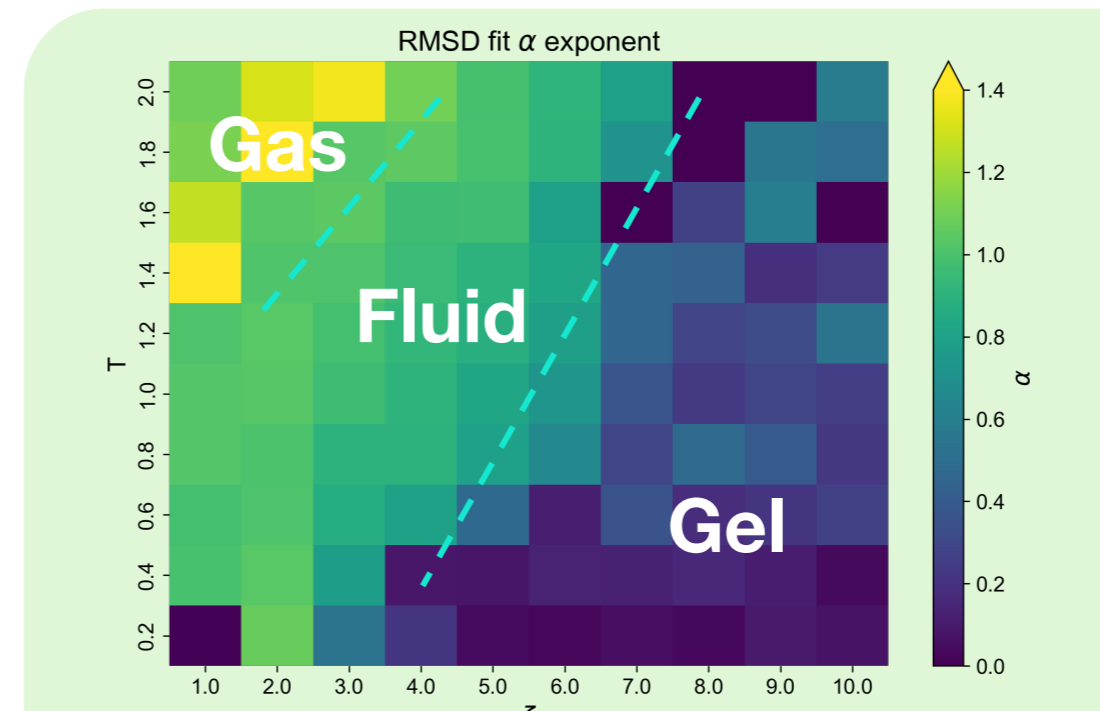
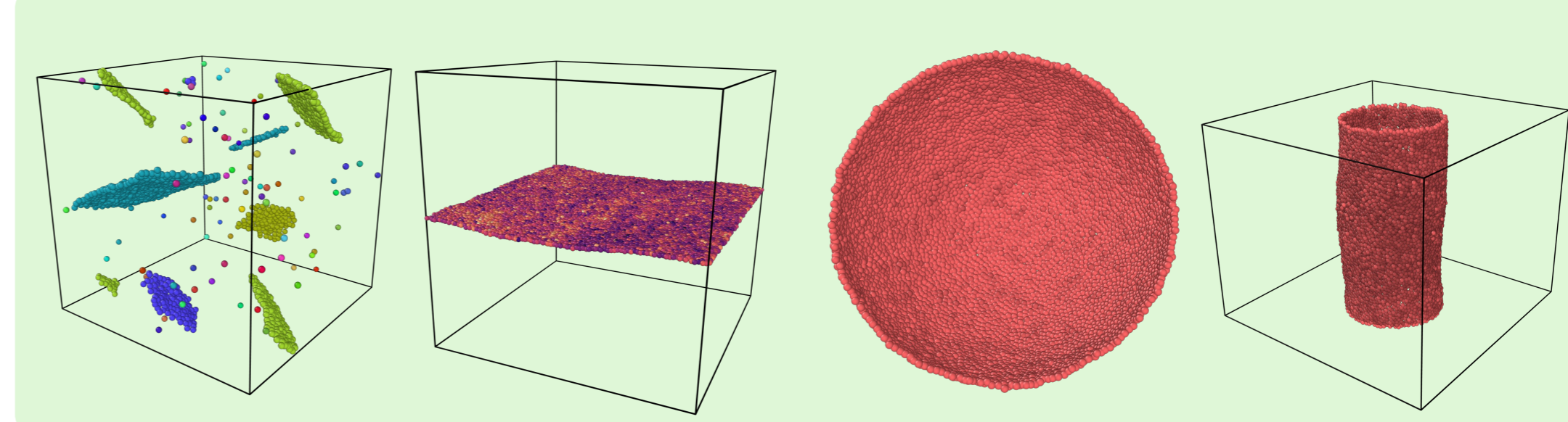
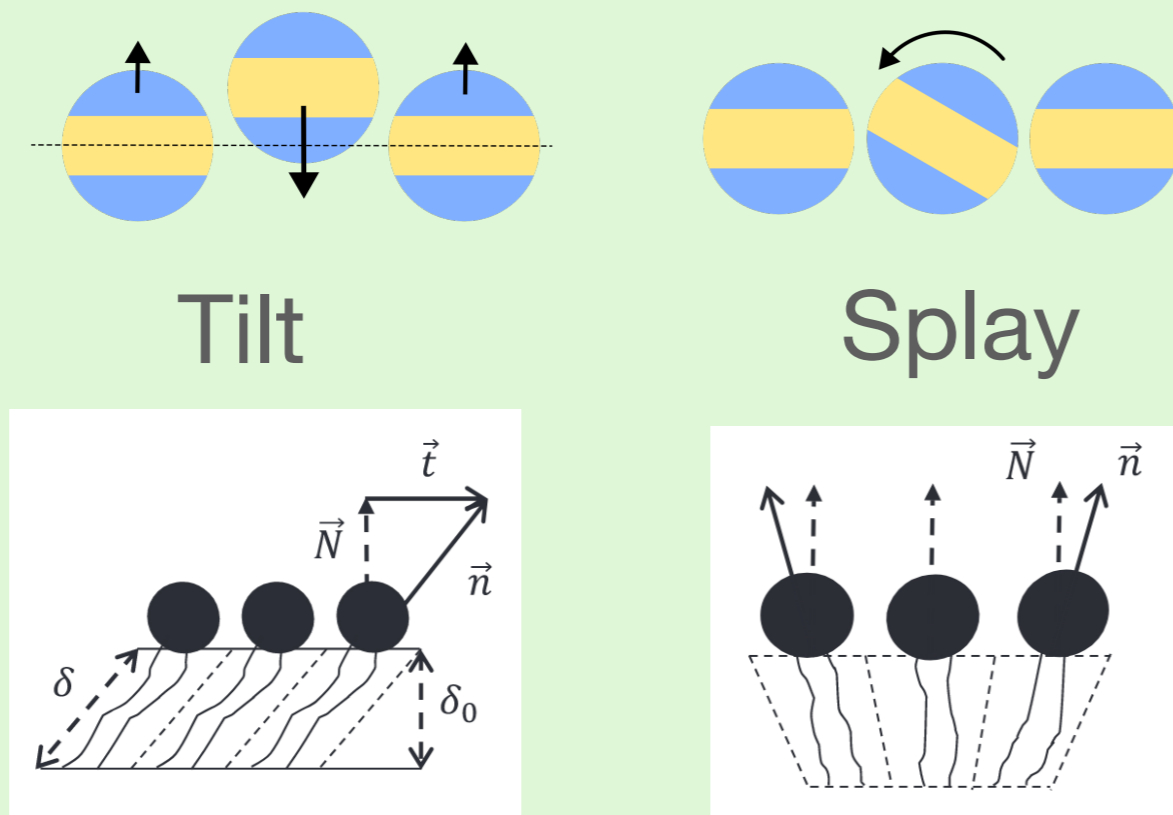
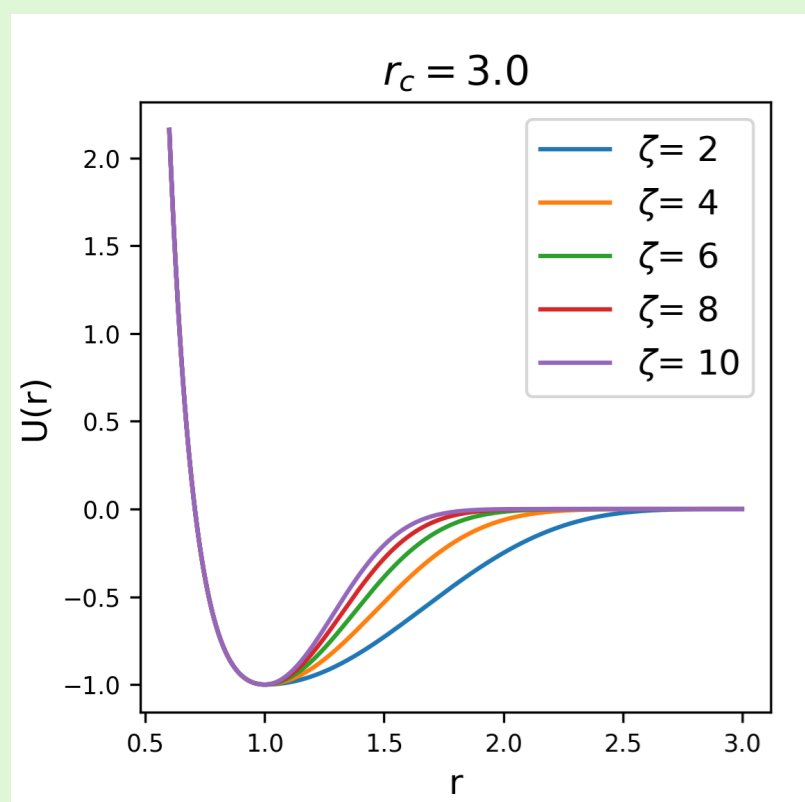
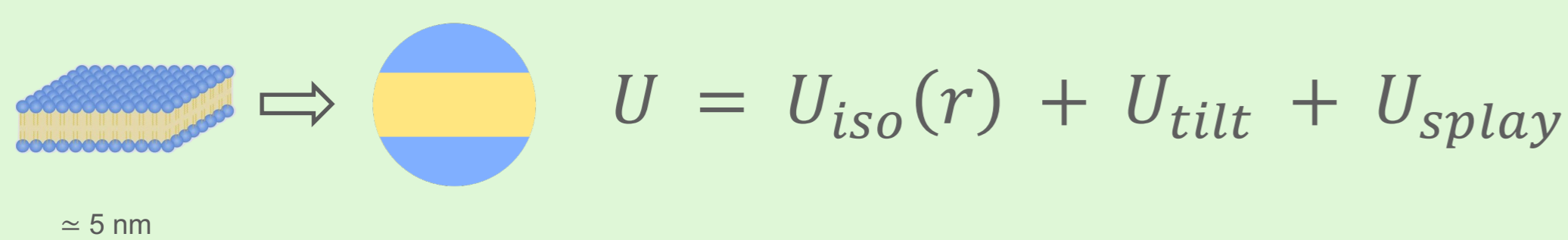


Microscopic \longrightarrow Macroscopic

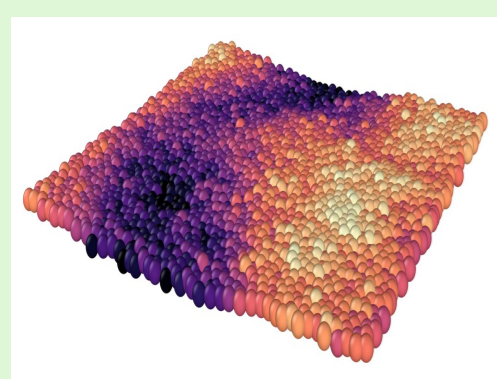
Can we develop a simple physics based model that allows for topology change and large deformations?

How do membranes mediate interactions?

Computational experiments can help us design and guide lab experiments.

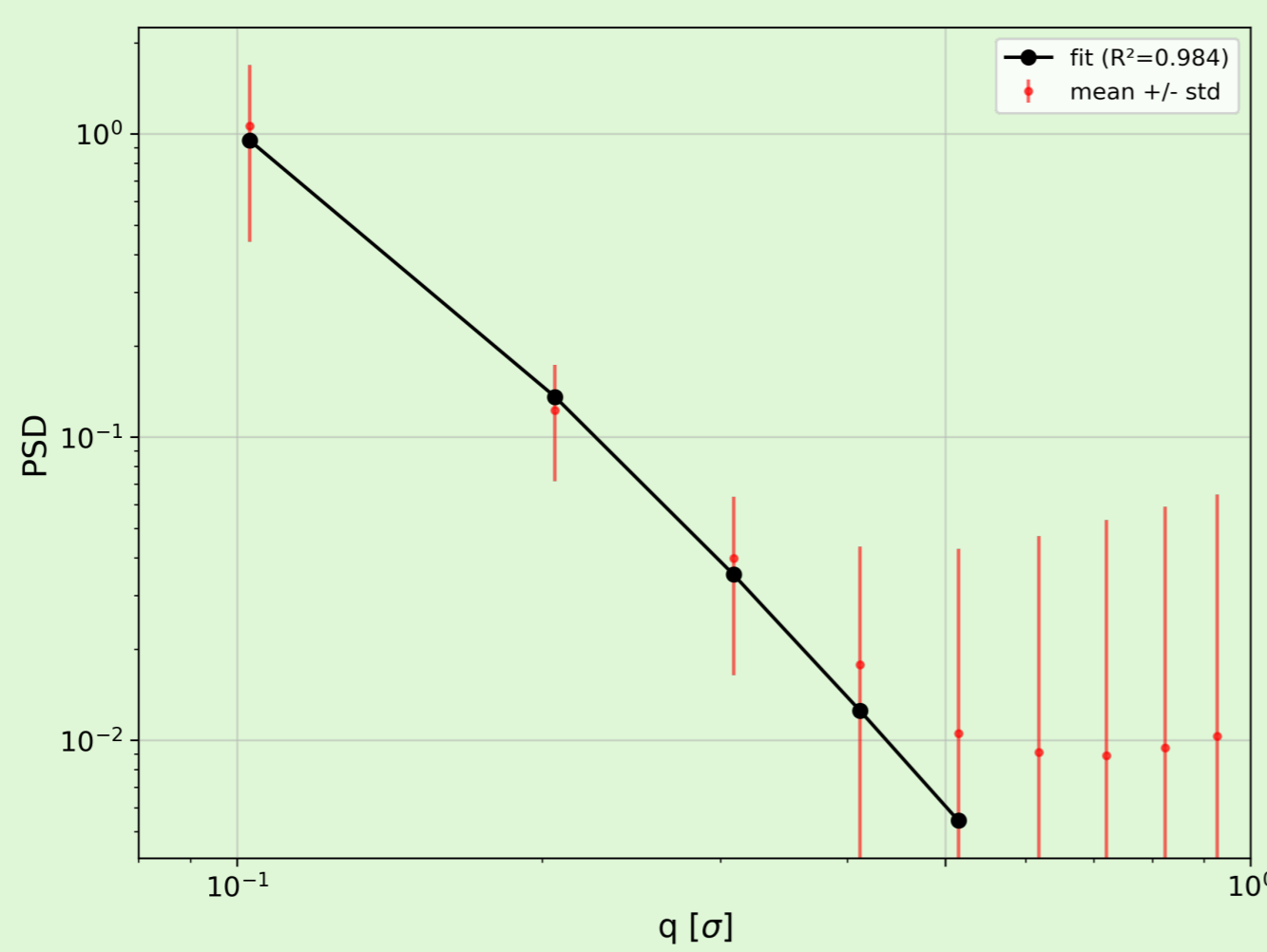


Implicit solvent \Rightarrow Langevin Dynamics
 Particles interaction $+$ Friction $+$ Thermal fluctuations

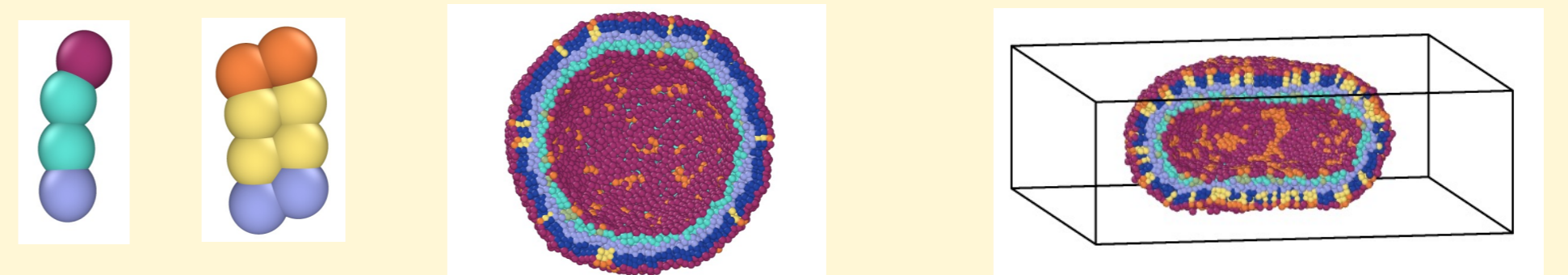


Fluctuation spectrum for a tension less membrane:

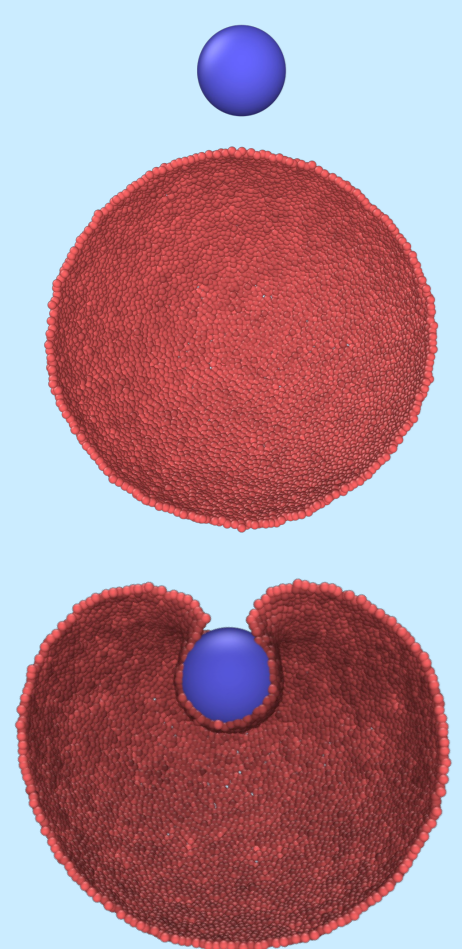
$$h(q) = \frac{K_b T}{L^2} k q^{-4}$$



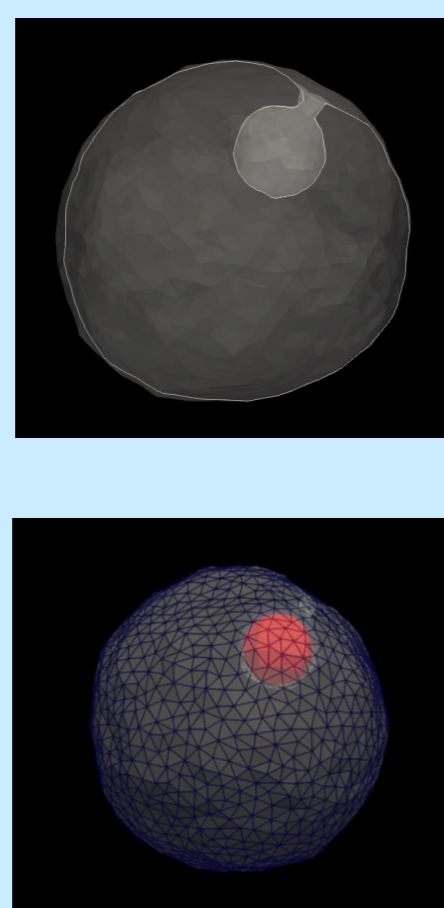
Curvature sensing properties of cardiolipins



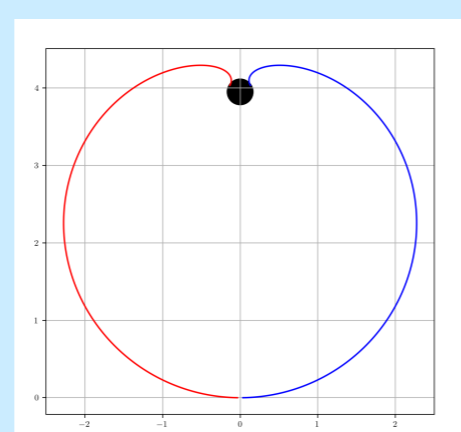
Endocytosis across methods



Particle based



Mesh based

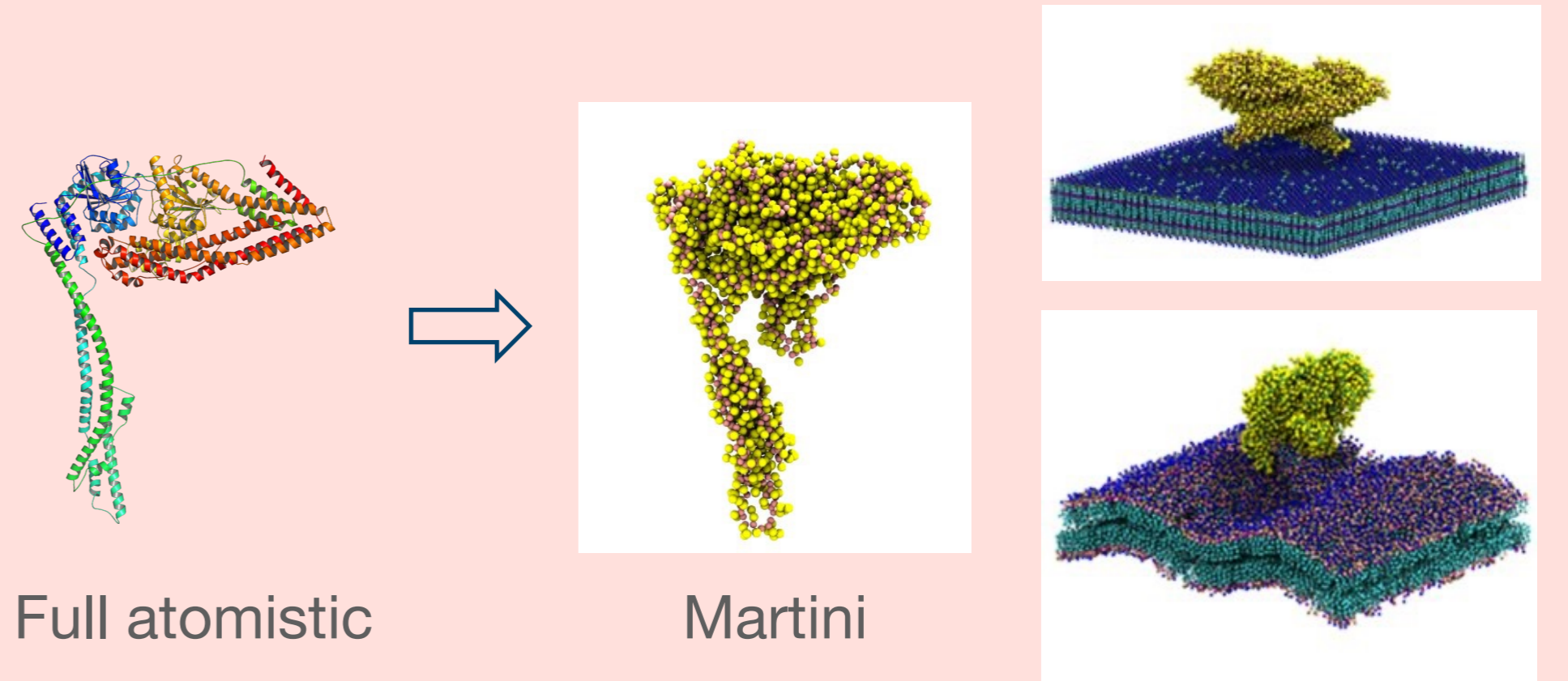


Shape minimizing E

$$E = E_{\text{bound}} + \int_{\text{bound}} dA(H^2 + \sigma)$$

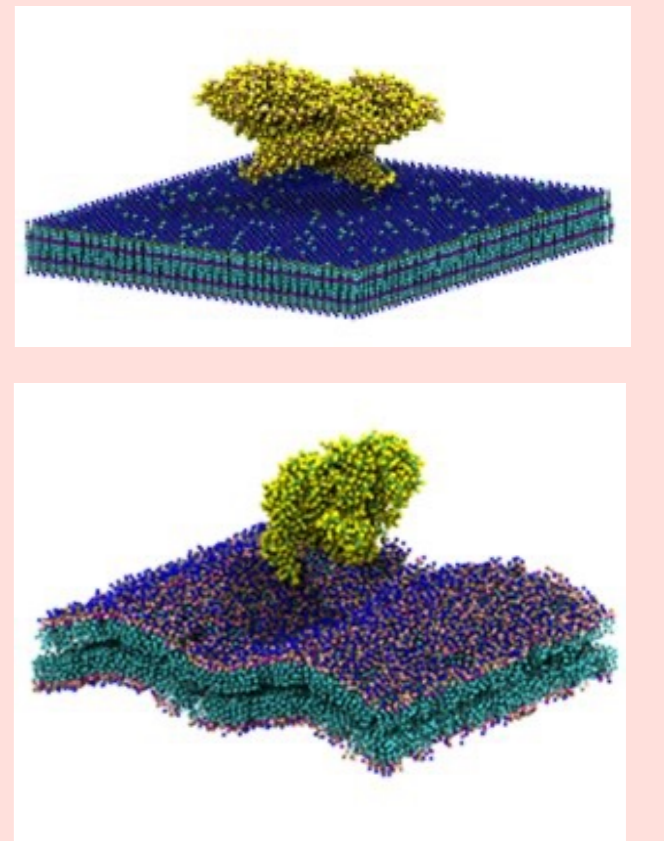
Continuum model

How does DynaminA sense membrane curvature?



Full atomistic

Martini



[1] SJ Marrink et al., "Martini 3", Nat Methods, 2021

[2] I. R. Cooke, K. Kremer, and M. Deserno, Phys. Rev. E, 2005

[3] W. Pezeshkian and J. H. Ipsen, "FreeDTS", Nat Commun, 2024



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FROM NON-LIFE TO LIFE