E1: Orders of magnitude

Week 5. Due Wed 10 Feb 23:59, reviewed Thu 11 Feb

About 2 hours. Submit one PDF (handwritten and scanned is fine) or a notebook on Canvas. You may use an LLM, but be ready to explain any answer at the board on Thursday.

1. Nelson

Nelson, *Biological Physics*: Your Turn 1a, Problems 1.3, 2.2 and 2.5.

The software and web sites named in Problems 2.2 and 2.5 are from 2002 and mostly gone. Use these instead:

- **2.2:** open each structure in the browser at `https://www.rcsb.org/3d-view/<code>`, for example rcsb.org/3d-view/1MBN. This is the Mol* viewer. To measure a distance, turn on selection mode, click two atoms, and open *Measurements*. For the rhinovirus (4rhv), choose the biological assembly, not the asymmetric unit.
- **2.5:** skip part (a); the micelle file is no longer online. Instead, estimate the radius of a spherical micelle of 65 dodecyl (C_{12}) surfactants. Each tail has volume 0.35 nm³ and is at most 1.67 nm long. For part (b), download the 128-lipid DPPC bilayer (`dppc.tar.gz`) from the CHARMM-GUI lipid archive and open `dppc_n128.pdb` in the Mol* viewer (*Open Files*). Measure the bilayer thickness between the phosphorus atoms of the two leaflets. The simulation box is 6.4 nm × 6.4 nm, with 64 lipids per leaflet: what is the area per lipid?

2. The thermal energy scale

Calculate k_BT at body temperature (37 °C) in J, eV, kJ/mol and pN · nm. Compare it with the energy of one ATP hydrolysis (about 20 k_BT in the cell) and with a covalent C–C bond (about 350 kJ/mol). What does the comparison tell you about which structures in the cell are stable against thermal motion?

3. Python warm-up: fit a line with an uncertainty

Generate synthetic data $y = at + b +$ noise with $a = 2$, $b = 0.5$, 30 points for $t \in [0, 10]$ and Gaussian noise with standard deviation 1. Fit a straight line and report $a \pm \delta a$. Repeat 1000 times with new noise and compare the spread of the fitted a with the δa from a single fit. Plot one data set with the fit.

Hint: `np.polyfit(t, y, 1, cov=True)` returns the covariance matrix of the parameters.