Problem set 3

Due November 10, 2026

1. The dataset `metan2_gr.txt` contains the pair correlation function, $g(r)$, of a pair of methane molecules in water at $T = 298\ K$ determined by means of molecular dynamics umbrella sampling calculations (Czaplewski et al., *Protein Sci.*, **2000**, 9, 1235-1245).

   (a) Scale $g(r)$ so that it tends to 1 at distances around 10 Å. Make a plot of the scaled $g(r)$ and describe the minima and maxima found there.

   (b) Based on the scaled $g(r)$, compute the radial pair-distribution function $\rho^{(2)}(r)$, make a plot of it and comment on the shape of the plot.

   (c) Based on normalized $g(r)$, compute the potential of mean force $W(r)$ of solvent-mediated interactions of two methane molecule in water. If necessary, shift $W(r)$ so that it is zero on average at distances around 10 Å. Express the PMF in kJ/(mol of pairs of methane molecules).

   (d) Compute the radial mean force profile, $\langle F(r) \rangle$ defined as $F(r) = -W'(r)$ (the prime is for the first derivative) and make a plot. You can use, e.g., fitting splines to smooth the force profile but this is not necessary. Express the force in pN/(pair of methane molecules). Clip the high forces at small distances to see the shape of the force profile at distances starting shortly before the contact minimum in $g(r)$.

   (e) Estimate the force necessary to pull apart two methane molecules that form a hydrophobic dimer in water. (Hint: search for the most negative force after the contact minimum.)