**memory effects for diffusion of methane in water**

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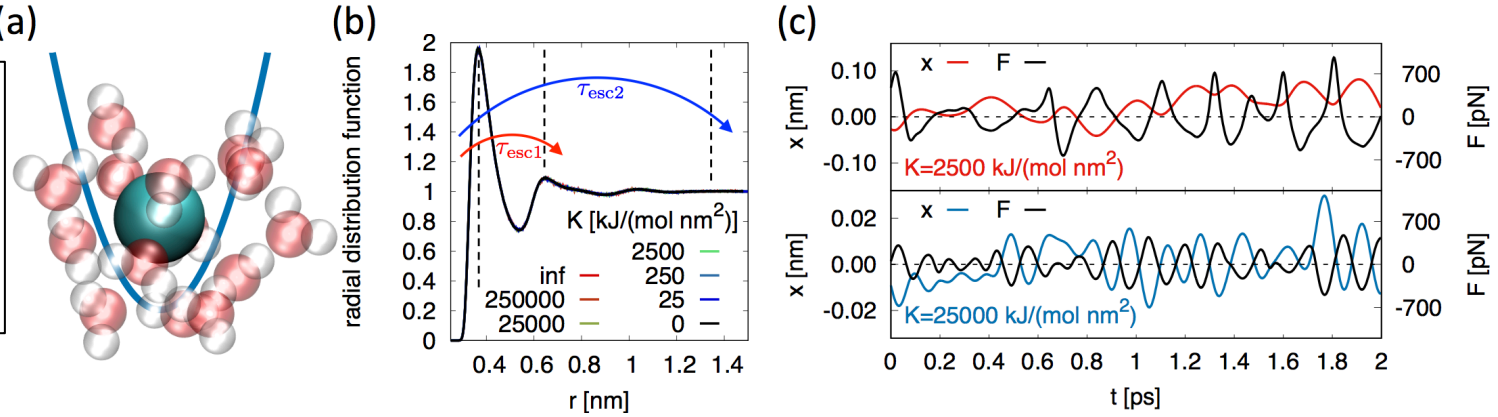


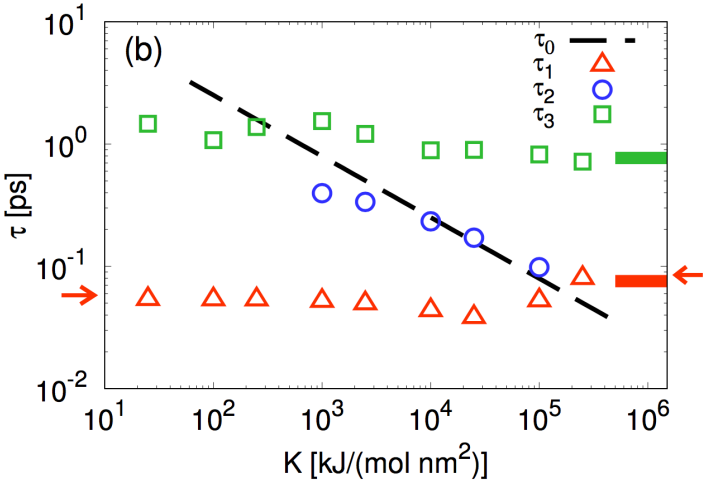

FIG. 1. **Simulation setup.** (a) A single methane is solvated in water and confined in an external harmonic potential of strength $K$. (b) Radial distribution function (RDF) of the separation between methane and water oxygens for box size $L = 4.5\,\mathrm{nm}$ and different $K$ including the frozen limit $K = \infty$, all curves perfectly superimpose. (c) Methane position $x(t)$ and total force $F(t)$ trajectories for two different $K$ values.

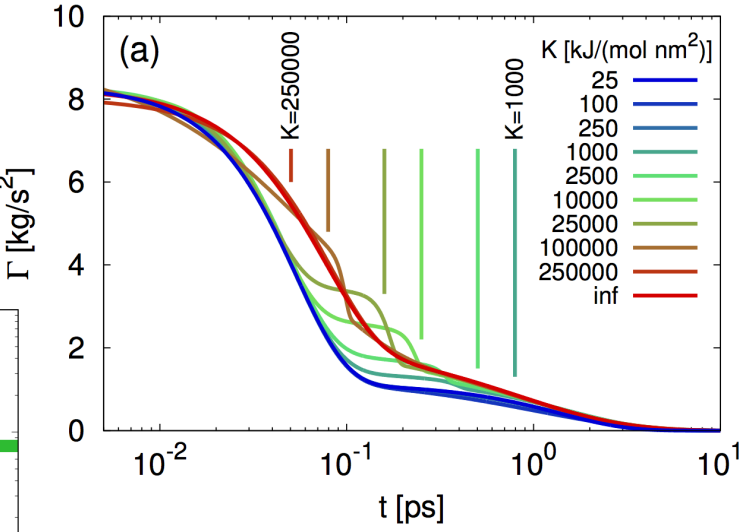
## mapping on inertial Langevin eq with memory

$$m\ddot{x}(t) = -\int_0^\infty dt'\,\Gamma(t')\dot{x}(t-t') - \nabla U(x(t)) + F_R(t),$$

$$U(x) = \tfrac{1}{2}Kx^2 \qquad \langle F_R(0)F_R(t)\rangle = k_B T\Gamma(t)$$

memory time scales




harmonic oscillation :

$$\tau_0 = 2\pi\sqrt{m/K}$$

fit function:

$$\Gamma(t) = \sum_{i=1}^{n} A_i \exp\left(-\left|\frac{t}{\tau_i}\right|^{\alpha_i}\right)$$