Temperature Echoes in Proteins

- Coherent motion in proteins: Echoes
- Generation of echoes in *ubiquitin* via velocity reassignments
  1) Temperature quench echoes
  2) Constant velocity reassignment echoes
  3) Velocity reassignment echoes

\[ T(t) = \frac{2}{(3N-6)k_B} \sum_{n=1}^{3N-6} \frac{m_n v_n^2(t)}{2} \]

**Generating T-Quench Echo: Step 1**

- your system is ubiquitin (1UBQ) in vacuum, pre-equilibrated at \( T_0 = 300K \)
- run all simulations in the *microcanonical* (NVE) ensemble
- psf, pdb and starting binary coordinate and velocity files are available in “common/”
- use NAMD2 configuration file “equil.conf” located in “01_equil_NVE/” to complete a 500 fs (# simulation steps) run
- extract the temperature time series \( T(t) \) from the NAMD2 log (output) file
- plot \( T(t) \)
- calculate: \( \langle T \rangle, \sqrt{\langle T^2 \rangle}, C_{TT} = \langle \delta T(t) \delta T(0) \rangle \)

**Temperature Autocorrelation Function**

\[ C(t) = \langle \Delta T(t) \Delta T(0) \rangle \]

\[ \rightarrow C(t) \approx \frac{1}{N-t} \sum_{n=1}^{N-t} \Delta T(t_{n+1}) \Delta T(t_n) \]

\[ C(t) = C(0) \exp \left( -t / \tau_0 \right) \]

Temperature relaxation time:

\[ \tau_0 \approx 2.2 \, \text{fs} \]

Mean temperature:

\[ \langle T \rangle = 299 \, \text{K} \]

RMS temperature:

\[ \sqrt{\langle \Delta T^2 \rangle} = \sqrt{C(0)} = 6 \, \text{K} \]

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**Generating T-Quench Echo: Step 2**

Perform the 1st temperature quench

- start a new simulation using configuration file “quench.conf” located in “02_quenchecho/”
- use the restart coordinate file from the previous run
- set all velocities to zero (i.e., set T=0)
- run the simulation for \( \tau \) number of steps (time step = 1 fs)
- extract (from the log file) and plot \( T(t) \)

Generating T-Quench Echo: Step 3

Perform the 2nd temperature quench
- start a new simulation using configuration file "quench.conf" located in "03_quenchb/"
- use the restart coordinate file from the previous run
- set again all velocities to zero (i.e., set T=0)
- run the simulation for 3\tau number of steps (time step = 1 fs)
- extract (from the log file) and plot T(t)

You should discover a temperature echo at 2\tau

Explanation of the T-Quench Echo

Assumption: protein \approx collection of weakly interacting harmonic oscillators with dispersion \omega = \omega_\alpha, \alpha = 1, \ldots, 3N - 6

Step 1: \ t < 0
\begin{align*}
x(t) &= A_0 \cos(\omega t + \theta_0) \\
v(t) &= -\omega A_0 \sin(\omega t + \theta_0)
\end{align*}

Step 2: \ 0 < t < \tau
\begin{align*}
x_1(t) &= A_1 \cos(\omega t + \theta_1) \\
v_1(t) &= -\omega A_1 \sin(\omega t + \theta_1)
\end{align*}
\Rightarrow \begin{cases} A_1 = A_0 \cos \theta_0 \\
\theta_1 = 0 \end{cases}

Step 3: \ t > \tau
\begin{align*}
x_2(t) &= A_2 \cos(\omega t + \theta_2) \\
v_2(t) &= -\omega A_2 \sin(\omega t + \theta_2)
\end{align*}
\Rightarrow \begin{cases} A_2 = A_1 \cos \omega \tau \\
\theta_2 = -\omega \tau \end{cases}

\[ T(t) \approx \frac{T_0}{4} \left[ 1 - \langle \cos(2\omega(t - \tau)) \rangle - \frac{1}{2} \langle \cos(2\omega(t - 2\tau)) \rangle \right] \]

\[ \approx \begin{cases} 
0 & \text{for } t = \tau \\
T_0/8 & \text{for } t = 2\tau \\
T_0/4 & \text{otherwise} 
\end{cases} \]

\[ \Rightarrow \text{echo depth} = T(2\tau) - \frac{T_0}{4} = \frac{T_0}{8} \]

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\[ T(t) \text{ and } C_{TT}(t) \]

It can be shown:

\[ \langle \cos(2\omega t) \rangle = \frac{\langle \delta T(t) \delta T(0) \rangle}{\langle \Delta T^2 \rangle} = C_{TT}(t), \quad \delta T(t) = T(t) - \langle T \rangle \]

Accordingly,

\[ T(t) \approx \frac{T_0}{4} \left[ 1 - \langle \cos(2\omega(t - \tau)) \rangle - \frac{1}{2} \langle \cos(2\omega(t - 2\tau)) \rangle \right] \]

\[ = \frac{T_0}{4} \left[ 1 - C_{TT}(t - \tau) - \frac{1}{2} C_{TT}(t - 2\tau) \right] \]

\[ T(t) \approx \frac{T_0}{2} \left( 1 - C_{TT}(t-\tau) - \frac{1}{2} C_{TT}(|t-2\tau|) \right) \]

\[ C_{TT}(t) = \exp(-t/\tau_0), \quad \tau_0 \approx 2.2 \text{ fs} \]


\[ \Delta T(\tau) = \Delta T(0) \exp\left[-\tau / \tau_{\text{dephase}}\right] \]