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

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

kinetic temperature:
Generating T-Quench Echo: Step 1

- your system is ubiquitin (1UBQ) in vacuum, pre-equilibrated at $T_0=300$K
- 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**

\[ \Delta T(t) = T(t) - \langle T(t) \rangle \]

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

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

\[ C(t) = C(0) \exp \left( -\frac{t}{\tau_0} \right) \]

Temperature relaxation time: \[ \tau_0 \approx 2.2 \text{ fs} \]

Mean temperature: \[ \langle T \rangle = 299 \text{ K} \]

RMS temperature: \[ \sqrt{\langle \Delta T^2 \rangle} = \sqrt{C(0)} = 6 \text{ K} \]
Generating T-Quench Echo: Step 2

Perform the 1st temperature quench
- start a new simulation using configuration file “quench.conf” located in “02_quencha/”
- use the restart coordinate file from the previous run
- set all velocities to zero (i.e., set T=0)
- run the simulation for τ 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 ≈ 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:** \( 0 < t < \tau \)

\[
\begin{align*}
x_1(t) &= A_1 \cos(\omega t + \theta_1) \\
v_1(t) &= -\omega A_1 \sin(\omega t + \theta_1)
\end{align*}
\]

\[
\begin{align*}
v_1(0) = 0 &\rightarrow \begin{cases} A_1 = A_0 \cos \theta_0 \\
\theta_1 = 0 \end{cases}
\end{align*}
\]

**Step 3:** \( t > \tau \)

\[
\begin{align*}
x_2(t) &= A_2 \cos(\omega t + \theta_2) \\
v_2(t) &= -\omega A_2 \sin(\omega t + \theta_2)
\end{align*}
\]

\[
\begin{align*}
v_2(\tau) = 0 &\rightarrow \begin{cases} A_2 = A_1 \cos \omega \tau \\
\theta_2 = -\omega \tau \end{cases}
\end{align*}
\]


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

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

$$\Rightarrow \text{echo depth} = T(2\tau) - T_0/4 = T_0/8$$
\[ T(t) \text{ and } C_{TT}(t) \]

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,

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

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


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

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