NAMD Tutorial (Part 2)

2 Analysis

2.1 Equilibrium
- 2.1.1 RMSD for individual residues
- 2.1.2 Maxwell-Boltzmann Distribution
- 2.1.3 Energies
- 2.1.4 Temperature distribution
- 2.1.5 Specific Heat

2.2 Non-equilibrium properties of protein
- 2.2.1 Heat Diffusion
- 2.2.2 Temperature echoes

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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

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

- are sharp, resonance-like features in the time evolution of the protein's temperature
- can be produced through 2 consecutive velocity reassignments


Producing Temperature Echoes by Velocity Reassignments in Proteins

Temperature quench echoes: \( v_i(0) = v_i(\tau) = 0 \)

Const velocity reassignment echoes: \( v_i(0) = v_i(\tau) = u_i \)

Generating T-Quench Echo: Step1

- 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

$\Delta T(t) = T(t) - \langle T(t) \rangle$

$C(t) = \langle \Delta T(t) \Delta T(0) \rangle$

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

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

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: Step2

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: Step3

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 3τ number of steps (time step = 1 fs)
- extract (from the log file) and plot T(t)

You should discover a temperature echo at 2τ
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: \( 0 < t < \tau \)
\[
\begin{align*}
x_1(t) &= A_1 \cos(\omega t + \theta_1) \\
v_1(t) &= -\omega A_1 \sin(\omega t + \theta_1)
\end{align*}
\]
\[v_1(0) = 0 \quad \Rightarrow \begin{cases} A_1 &= A_0 \cos \theta_0 \\ \theta_1 &= 0 \end{cases} \]

Step 3: \( t > \tau \)
\[
\begin{align*}
x_2(t) &= A_2 \cos(\omega t + \theta_2) \\
v_2(t) &= -\omega A_2 \sin(\omega t + \theta_2)
\end{align*}
\]
\[v_2(\tau) = 0 \quad \Rightarrow \begin{cases} A_2 &= A_1 \cos \omega \tau \\ \theta_2 &= -\omega \tau \end{cases} \]


T-Quench Echo: Harmonic Approximation

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

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

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

$T(t)$ and $C_{TT}(t)$

It can be shown:

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

Accordingly,

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

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


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**T-Quench Echo: Harmonic Approximation**

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

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

**Dephasing Time of T-Quench Echoes**

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


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**Constant Velocity Reassignment Echo?**

Can we get temperature echo(es) by reassigning the same set of atomic velocities (corresponding to \( T_0 \)) at \( t = 0 \) and \( t = \tau \)?

\[
v_i(0^+) = v_i(\tau^+) = u_i, \quad i = 1, ..., 3N - 6
\]

Answer: YES!

\[
T(t) \approx T_0 \left[ 1 - \frac{1}{2} C_{TT} \left( |t - 3\pi/2| \right) \right]
\]