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

Main funding:
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:
**Temperature Autocorrelation Function**

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

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

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

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

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 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 (number of simulation steps) run
- Extract the temperature time series $T(t)$ from the NAMD2 log (output) file
- Plot $T(t)$
- Calculate: $\langle T \rangle$, $\sqrt{\langle T^2 \rangle}$, $C_T = \langle \delta T(t) \delta T(0) \rangle$
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
Explantion of the T-Quench Echo

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

Step 1: \( t < 0 \)
\[ x(t) = A_0 \cos(\omega t + \theta_0) \]
\[ v(t) = -\omega A_0 \sin(\omega t + \theta_0) \]

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

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

Accordingly, 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,

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

\[\downarrow\]

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

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

$\nu_i(0^+) = \nu_i(\tau^+) = u_i, \ i = 1, \ldots, 3N - 6$

Answer: YES!

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