Analysis of BPTI Equilibrium Properties

Ioan Kosztin

Beckman Institute
University of Illinois at Urbana-Champaign

Formulation of the Problem

The minimized structure of the *Bovine Pancreatic Trypsin Inhibitor* (BPTI) protein was equilibrated at T=300K for 200ps by using NAMD2. The coordinate (velocity) PDB file corresponding to the end of the equilibration process is **bpti_equil.coor** (**bpti_equil.vel**). This state served as initial condition for two MD runs, 200ps long each, the 1st corresponding to the NEV ensemble (free dynamics), and the 2nd to the NTV ensemble (langevin dynamics). The corresponding configuration, output and DCD trajectory (for both coordinates and velocities) are as follows.

free.namd		lang.namd
free.out	and	lang.out
bpti_free.dcd		bpti_lang.dcd
bpti_free_vel.dcd		bpti_lang_vel.dcd

Our goal is to analyze these MD trajectories, i.e., to extract useful properties/information about the protein system by employing some freely available computational tools (software).

Suggested Tasks

• Get information about the simulation by inspecting the **configuration** and **output** files

• Using **namdplot** and the **output** files, graph the time dependence of the different energy components and the (kinetic) temperature

• Using **xmgrace** (or otherwise) determine the **mean** and **RMS** (standard) **deviation** of the total (*E*), kinetic (*K*) and potential (*U*) energies

• Use the obtained results to determine the specific heat capacity C_v and check the validity of the formulas: $T = \frac{2}{3Nk_B}\langle K \rangle_{NVT}$

$$\langle \delta K^2 \rangle_{NVT} = \frac{3N}{2}(k_B T)^2$$

$$\langle \delta U^2 \rangle_{NVT} = k_B T^2 (C_V - 3Nk_B/2)$$

Load one of the coordinate DCD files into VMD and using the features of this program

• Graph the *t*-dependence of the end-to end distance of BPTI (e.g., distance between the terminal C^α atoms)

• Calculate and graph the *t*-dependence of the **radius of gyration** of the BPTI molecule

Suggested Tasks (cont.)

• Calculate the **MSD** of the **backbone atoms** of BPTI between the **first** and **last frame** of the simulation (align first!)

• Calculate and plot the **time average** of the **RMSD** of **each residue** of the BPTI (align with the first frame!)

• Calculate the **Debye-Waller Factors** corresponding to the C^α atoms

• Calculate the total charge ***Q*** and dipole moment ***P***(*t*) of the system

• Calculate and graph the **dipole moment autocorrelation function**

Load one of the velocity DCD files in VMD and

• Check the validity of the formula

$$T = 2K/3Nk_B$$

• Calculate and plot the **velocity autocorrelation function** of one of the C^α atoms