Using the velocity auto-correlation function to characterize functional "noise" in bio-molecules

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Characterization of noise in simulated electrical systems often relies on the Fourier transform of the auto-correlation function of the velocity, or the fluctuation of the velocity, of electrons. This same approach can also be used in the simulations of other systems such as the simulation of biological systems, which relies on a statistical mechanics description through the calculation of the trajectories of the atoms over time.

In the simulation of bio-molecules, the position and velocity of each atom is recorded every $\Delta t$. This allows us to characterize what we can call molecular "noise", that is in fact how the molecules vibrate. When calculating the Fourier transform of the auto-correlation function of the velocities of the atoms of a bio-molecule, we gain access to its vibrational density of states as in figure 1, which can then directly be compared to experimental spectra such as the THz spectra of the same bio-molecule. Through this approach, we can couple simulation and experiments to gain insights into this molecule’s signature molecular vibrations which can be important from a biological and physical point of view.

Fig. 1. Vibrationnal density of state of the model protein Bovine Serum Albumin (PDB ID: 3V03).

REFERENCES