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FB Mathematik und Informatik

Computational Molecular Physics **Winter 2017/18**

Problem set 8 — 12 January 2018

Problem 8.1 *Brownian motion in a harmonic trap: correlation functions*

The ASCII files `trajectory_8-[1-3].dat` contain trajectories of three different diffusing particles. Each column is a time series $x_i(t)$ of one Cartesian coordinate ($i = 1, 2, 3$), sampled at the time intervals Δt given in the first line. The columns within the same file may be considered independent measurements of the same situation.

a) For each dataset, calculate the mean-square displacement $\delta r^2(t) = \sum_i \langle |x_i(t) - x_i(0)|^2 \rangle$ from a time average. Use the naïve nested-loop algorithm and restrict to the first 10^4 or 10^5 data points for performance reasons. Plot your results on double-logarithmic scales and in a single figure, add a legend.

b) Calculate the power spectral density $S(\omega)$ using fast Fourier transformation (FFT) for frequencies $\omega = 2\pi n/T$, where $n = 0, \dots N/2$ and $T = N\,\Delta t$ is the length of the trajectory. Process each Cartesian coordinate separately. Apply the Wiener–Khinchin theorem to obtain an estimate for $\delta r^2(t)$.

Hint: FFT is efficient only if the length of the input data is of the form $2^k 3^l 5^m$ for $k, l, m = 0, 1, 2, \dots$

c) Implement a multiple-τ correlation algorithm as described in the lecture. Use blocks of length $\ell = 10$ and as many levels as required to cover correlation times of $T/10$. Calculate $\delta r^2(t)$ for the full data sets and compare with your findings from the previous methods.

Hint: For performance reasons, it is advised to restrict the calculation of short-time correlations suitably, e.g., by requiring a minimal separation of initial points $x_i(t_0)$.

d) Depending on the dataset, the results for $\delta r^2(t)$ should exhibit some or all of the following regimes:

$$\delta r^2(t) \simeq \begin{cases} \langle v^2 \rangle t^2, & \text{inertial or ballistic motion,} \\ 6Dt, & \text{free diffusion,} \\ \ell^2, & \text{localisation or confined motion.} \end{cases}$$

Identify time windows in your data, where such behaviour is observed, and determine the parameters $\langle v^2 \rangle$, D, ℓ.

e*) Compute the velocity autocorrelation function $Z(t)$ by *(i)* correlating the increments of the time series (differences of adjacent samples) and *(ii)* taking a second derivative of $\delta r^2(t)$ using central difference quotients. Plot your results using a logarithmic time axis. Can you identify exponential decays, $Z(t) \sim \mathrm{e}^{-t/\tau}$, or sums thereof?

Due date: ***19 January, 6 p.m.***