Time Correlation Function

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Introduction

Correlation Functions

Correlations between two different quantities A and B are measured in the usual statistical sense, via the **correlation coefficient**: c_{AB}

$$c_{AB} = \langle \delta A \delta B \rangle / (\sigma(A)\sigma(B))$$

$$\delta X = X - \langle X \rangle_{ens}$$

- Schwartz inequalities guarantee that the absolute value of c_{AB} lies between 0 and 1, with values close to 1 indicating a high degree of correlation
- Considering A and B to be the same quantity evaluated at different times we can obtain an **Autocorrelation function**: $c_{AA}(t)$

Introduction

Autocorrelation Function

The non-normalized autocorrelation function is defined: $C_{AA}(t)$

$$C_{AA}(t) = \langle \delta A(t) \delta A(0) \rangle_{ens} = \langle \delta A(\Gamma(t)) \delta A(\Gamma(0)) \rangle_{ens}$$

then the coefficient("normalized autocorr. funct.") is:

$$c_{AA}(t) = C_{AA}(t)/\sigma^2(A) = C_{AA}(t)/C_{AA}(0)$$

$$\sigma^2(A) = \langle \delta A^2 \rangle_{ens} = \langle A^2 \rangle_{ens} - \langle A \rangle_{ens}^2$$

- You can calculate time correlation functions from a file that contains the mechanical property of interest $A(t)$ stored at regular intervals during a molecular dynamics (MD) simulation

Introduction

$$c_{AB} = \langle \delta A \delta A / \sigma^2(A) \rangle$$

- They give a clear picture of the dynamics in a fluid
- Their time integrals t_A may often be related directly to macroscopic transport coefficients
- Their Fourier transforms $\hat{c}_{AA}(\omega)$ may often be related to experimental spectra measured as a function of frequency ω.

$$\sigma^2(A) = \langle \delta A^2 \rangle_{ens} = \langle A^2 \rangle_{ens} - \langle A \rangle_{ens}^2$$

Calculations

Direct Approach

- $A(t)$ will be available at equal intervals of time δt
- δt is a small multiple of the timestep: $t = \tau \delta t$

The discretized form will be then:

$$C_{AA}(\tau) = \langle A(\tau)A(0) \rangle = \frac{1}{\tau} \sum_{\tau_0=1}^{\tau_{max}} A(\tau_0)A(\tau_0 + \tau)$$

- We average over τ_{max} time origins the product of A at time $\tau_0 \delta t$ and A at a time $\tau \delta t$ later
- For each value of τ, the value of $\tau_0 + \tau$ must never exceed the number of values of A , τ_{run}, stored in the file
- Thus, the short-time correlations, with τ small, may be determined with slightly greater statistical precision because the number of terms in the average, τ_{max} may be larger