Error estimates and variance reduction for transport coefficients

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Equilibrium properties in statistical physics are obtained by computing averages with respect to Boltzmann--Gibbs measures, sampled in practice using ergodic dynamics such as the Langevin dynamics. Some quantities however cannot be computed by simply sampling the Boltzmann--Gibbs measure, in particular transport coefficients, which relate the current of some physical quantity of interest with the forcing needed to induce it. For instance, a temperature difference induces an energy current, the proportionality factor between these two quantities being the thermal conductivity. From an abstract point of view, transport coefficients can also be considered as some form of sensitivity analysis with respect to an added forcing to the baseline dynamics.

There are various numerical techniques to estimate transport coefficients, which all suffer from large errors, in particular large statistical errors. I will review the most popular methods, namely the Green--Kubo approach where the transport coefficient is rewrittten as some time-integrated correlation function, and the approach based on longtime averages of the stochastic dynamics perturbed by an external driving (so-called nonequilibrium molecular dynamics). I will make precise in each case the various sources of errors, in particular the bias related to the time discretization of the underlying continuous dynamics, and the variance of the associated Monte Carlo estimators. I will also briefly present various recent alternative techniques to estimate transport coefficients.