M2 internship (+ PhD) “Efficient computation of linear response of nonequilibrium stochastic dynamics”

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I describe the topic for a 4 to 6 month internship – but in fact the many questions raised by the approach proposed in this document transform the description below into a proper PhD project. I already benefit from a PhD fellowship through the ANR SINEQ, which was accepted in 2021 and starts in 2022. A successful M2 intern is therefore guaranteed to be funded for a PhD. Overall, I am looking for an intern who is looking for a PhD project with some balance between deterministic and stochastic aspects, and between theoretical studies and the development of numerical methods.

1. Motivations and scientific context

Computational statistical physics (also known as molecular dynamics [4, 9]) can be seen as the numerical realization of the general philosophy of classical statistical physics, which allows in principle to obtain quantitatively accurate predictions on the behavior of materials once the interaction laws between atoms are given. These laws are defined by a potential energy function \( V(q) \), where \( q = (q_1, \ldots, q_N) \) is the microscopic configuration of a system of \( N \) atoms. Equilibrium properties are obtained as averages with respect to the high-dimensional probability measure describing the state of the system, which is defined in terms of \( V \). These averages are estimated in practice by sampling the measure of interest with runs of a Monte Carlo method, for instance a time discretization of a stochastic differential equation (SDE) ergodic for the target probability measure, and computing large time averages over a realization of the dynamics [7].

By default physical systems are out of equilibrium: they are subjected to external forcings, with energy or mass coming in and out. The associated microscopic dynamics, known as nonequilibrium molecular dynamics [1, 3], include external drivings such as non-conservative forces, and are therefore irreversible. The invariant probability measure (provided it exists and is unique) depends sensitively on the details of the dynamics, and is usually not known analytically. This prevents resorting to the standard variance reduction techniques used for equilibrium systems for which an a priori known expression of the invariant measure is needed. New dedicated numerical methods have therefore to be devised.

**Definition of transport coefficients.** Some quantities of prime interest in statistical physics are transport coefficients, which are obtained by an analogy with macroscopic thermodynamics, where transport coefficients are defined as the proportionality constant (or matrix) relating the current of some physical quantity of interest with the forcing needed to induce it. For instance, a temperature difference induces an energy current. At the microscopic level, the relevant framework is linear response theory [5]. To give an example, consider the estimation of the mobility [8, 6], defined as the proportionality factor between a constant force applied to a particle and its resulting average velocity: for a particle of position \( q \) in \( T^d = (\mathbb{R}/\mathbb{Z})^d \), the \( d \)-dimensional unit torus, and associated momentum \( p \) in \( \mathbb{R}^d \),

\[
\alpha = \lim_{\eta \to 0} \frac{E_\eta(\mathcal{J})}{\eta} = \beta \int_0^{+\infty} E_0 \left[ \mathcal{J} \left( q_t^0, p_t^0 \right) \mathcal{J} \left( q_0^0, p_0^0 \right) \right] dt, \quad \mathcal{J}(q,p) = F \cdot p, \tag{1}
\]

where \( \beta > 0 \) is proportional to the inverse temperature, \( F \in \mathbb{R}^d \) is a given forcing direction, and \( E_\eta \) is the expectation with respect to the invariant probability measure \( \mu_\eta \) of the following nonequilibrium
Langevin process with external forcing of magnitude $\eta \in \mathbb{R}$ and friction coefficient $\gamma > 0$: 

$$dq_t^\eta = p_t^\eta, \quad dp_t^\eta = \left(-\nabla V(q_t^\eta) + \eta F\right)dt - \gamma p_t^\eta dt + \sqrt{2\gamma\beta^-1}dW_t, \tag{2}$$

with $W_t$ a standard $d$-dimensional Brownian motion. Let us emphasize that the drift of the above dynamics is not the gradient of a periodic function, so that, in general, the invariant probability measure $\mu_\eta$ is not known for $\eta \neq 0$; whereas $\mu_0(dq dp) = Z^{-1}e^{-\beta H(q,p)}dq dp$ with $H(q, p) = V(q) + p^2/2$ the Hamiltonian of the system.

### Computation of transport coefficients.

Transport coefficients such as $\alpha$ in (1) are typically estimated by

- either approximating the time-integral in the second equality of (1) (Green–Kubo formula). Properly estimating this time integral is however challenging because the integrand is a correlation term which is very difficult to reliably estimate for long times, since it is a small quantity plagued by a large relative statistical error.

- or approximating the limit in the first equality of (1) by the finite difference $E_{\eta_\ast}(J)/\eta_\ast$ (with $\eta_\ast$ sufficiently small to limit the bias), and next estimating the expectation with time averages:

$$\hat{\alpha}_{t,\eta_\ast} = \frac{1}{\eta_\ast} \int_0^t J(q_{s_\ast}^\eta, p_{s_\ast}^\eta) \, ds. \tag{3}$$

For small values of $\eta_\ast$, the variance of the estimator $\hat{\alpha}_{t,\eta_\ast}$ scales as $\sigma^2/(\eta_\ast^2 t)$, where $\sigma^2$ is the asymptotic variance of trajectorial averages of the current $J$ at equilibrium ($\eta = 0$). The simulation time required to estimate $\alpha$ with a sufficient statistical accuracy therefore scales as $t \sim \eta_\ast^{-2}$, which is often prohibitive in practical cases of interest.

Although many practitioners of molecular dynamics realize that the computation of transport coefficients is a difficult numerical issue, there were only a handful of attempts to develop dedicated variance reduction techniques. Many practitioners still use direct, brute force numerical methods based on a time integration of the dynamics.

### 2. Aim of the internship/PhD project

The aim of the internship (and the subsequent PhD) is to study an alternative approach to simulating nonequilibrium systems, relying on a dual viewpoint: instead of fixing the forcing and measuring the average response of the system, one could alternatively fix the response and compute the average forcing needed to induce it (see Figure 1 for a schematic representation of this idea). This amounts to considering constrained dynamics with Lagrange multipliers chosen such that the current $J$ is constant. Transport coefficients would then be defined as the ratio of the fixed flux $J$ and the average forcing. This approach is known as Norton dynamics in the physics literature [3], and was numerically shown to be correct for the computation of the mobility for deterministic dynamics [2]. As promising as they seem, Norton dynamics have not been studied from a mathematical viewpoint, and their numerical efficiency has not yet been assessed. One of the challenges is that the current constraint is not holonomic, so that the projection of Langevin-type stochastic dynamics onto the submanifold of constant current configurations has to be defined properly. The forcing should in any case extend to the whole system, and not only arise from the boundaries.

In order to provide a convenient mathematical analysis, the first step is to extend the Norton philosophy to stochastic dynamics and provide clear criteria to determine which forcings can be used to fix the current. The next step is to study the properties of the resulting dynamics, both from theoretical and numerical perspectives: (i) show that it is well posed and that it admits a unique invariant measure; (ii) prove that a transport coefficient can be defined from the linear response of averages under this invariant measure; (iii) show the consistency of the Norton approach with the standard definition of transport coefficients (1) in the thermodynamic limit where the number of particles goes to infinity, at least for model systems (atom chains with harmonic interactions); (iv) perform the numerical analysis of the method; (v) numerically quantify the performance of the method.
Figure 1: Schematic representation of the idea of Norton systems: instead of fixing the forcing and monitoring a fluctuating response as usually done (left), one fixes the response of the system and monitors the forcing needed to induce it (right).

References


