Optimal prediction and the Mori-Zwanzig representation of irreversible processes

Alexandre J. Chorin
Ole H. Hald

Department of Mathematics
Lawrence Berkeley National Laboratory
1 Cyclotron Road, Berkeley CA 94720

Raz Kupferman

Institute of Mathematics
The Hebrew University
Jerusalem 91904 Israel

Abstract

Optimal prediction methods compensate for a lack of resolution in the numerical solution of complex problems through the use of prior statistical information. We point out a relation between optimal prediction and the statistical mechanics of irreversible processes, and use a version of the Mori-Zwanzig formalism to produce a higher-order optimal prediction method.

1 Introduction

Many problems in science and engineering are described by nonlinear equations whose solutions are too complicated to be properly resolved. The problem of predicting the evolution of systems that are not well resolved has been addressed by the present authors and others in [1, 2, 3, 4]. Nothing can be predicted without *some* knowledge about the unresolved ("subgrid") degrees of freedom. In the optimal prediction methods of [1, 2, 3, 4] it is assumed that one possesses, as one often does, prior statistical information about the system in the form of an invariant measure; what is sought is a mean solution with respect to this prior measure, compatible with the information initially at hand as well as with the limitations on the computing power one can bring to bear.

In principle, finding the mean solution requires the solution of a Liouville equation: an equation for a probability measure on the space of solutions. To solve the Liouville equation is in general even harder than to solve the original problem. In optimal prediction methods one calculates means with respect to the invariant measure conditioned by the available data. This approximation yields a reduced set of equations for a system of "collective variables". A rigorous analysis can be found in [5].

The simplest version of this idea, first-order optimal prediction, generates an approximating system of ordinary differential equations and works well for a time that depends on the number of collective variables and on the temperature, i.e., the variance of the initial data. Even though this approximation is optimal, in a sense explained below, it eventually exhibits errors, because the influence of partial initial data on the distribution of the solutions weakens in time if the system is ergodic, and this loss of information is not captured in full, see [4].

The present paper is a step towards higher-order optimal prediction methods that are accurate for longer times. We point out a relation between underresolved computation and nonequilibrium statistical mechanics; this relation suggests that methods used in the latter are applicable also to the former. Of particular interest is the work of Mori [6] and Zwanzig [7] (see also [8]) which relates the evolution of macroscopic variables to microscopic dynamics. The Mori-Zwanzig theory gives rise to a generalized Langevin equation for a set of collective variables; if one observes the evolution of a system through a projection on a subset of its degrees of freedom, the evolution of the selected variables can be viewed as the sum of a deterministic part and a random, "noisy" part; the randomness reflects one's ignorance of unresolved degrees of freedom. This theory has been known for decades in the context of transport theory, but its relevance to underresolved differential equations is a novel idea.

The standard Mori-Zwanzig theory has been given a nonlinear generalization by Zwanzig [7]. First-order optimal prediction coincides with Zwanzig's generalization when random and non-Markovian "memory" effects are small. Zwanzig's equation is an identity, and allows, at least in principle, a better assessment of the errors in various approximations.

In Section 2 we derive the generalized Langevin equation and compare it with first-order optimal prediction. Our derivation is more general than Zwanzig's and not limited to Hamiltonian dynamics. In Section 3 we apply the theory to the nonlinear Schrödinger equation that was studied in [2, 4], and derive expressions for the noise and the memory kernel by perturbative methods. We show that the inclusion of memory effects predicts the loss of information in long time numerical integrations. The analogy between irreversible statistical mechanics and underresolved computation is the main contribution of the present paper.

2 Phase variables and the Mori-Zwanzig formalism

Consider a problem of the form

$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{R}(\boldsymbol{u}), \tag{2.1}$$

where $\boldsymbol{R}$ and $\boldsymbol{u}$ are n-dimensional vectors (n may be infinite), with components R_i and u_i, and t is the time. When n is finite (2.1) is a system of ordinary differential equations.

We denote the phase space (the vector space in which $\boldsymbol{u}$ resides) by $\boldsymbol{\Gamma}$; in classical statistical physics this phase space is the $n = 6\ell$ dimensional space of coordinates and momenta, (q_i, p_i), where ℓ is the number of particles. A solution of equation (2.1) is defined when an initial value $\boldsymbol{u}(t=0) = \boldsymbol{u}_0$ is given; to each initial condition $\boldsymbol{u}_0$ corresponds a trajectory, $\boldsymbol{\varphi}(t) = \boldsymbol{\varphi}(\boldsymbol{u}_0, t)$. From now on, we omit the subscript 0; $\boldsymbol{u}$ (without argument or subscript) is always the initial state of the system, and $\boldsymbol{\varphi}(\boldsymbol{u}, t)$ is the state of the system at time t.

A phase variable A is a function on $\boldsymbol{\Gamma}$, in general vector-valued; when A has m components, we denote them by A_i, $i = 1, \ldots, m$. A phase variable varies when its argument varies in time, so that a phase variable whose value at $t = 0$ was $A(\boldsymbol{u})$ acquires at time t the value $A(\boldsymbol{\varphi}(\boldsymbol{u}, t))$. One can also take a "Heisenberg" or "Lagrangian" point of view and introduce a time-dependent phase variable $S^t A$, where S^t is a time evolution operator for phase variables, defined through the relation

$$(S^t A)(\boldsymbol{u}) = A(\boldsymbol{\varphi}(\boldsymbol{u}, t)). \tag{2.2}$$

(Remember that in this equation $\boldsymbol{u}$ is an initial state.) Differentiation of (2.2) with respect to time and use of the identity $\boldsymbol{R}(\boldsymbol{\varphi}(\boldsymbol{u}, t)) = \nabla_{\boldsymbol{u}} \boldsymbol{\varphi}(\boldsymbol{u}, t) \cdot \boldsymbol{R}(\boldsymbol{u})$ yields

$$\frac{\partial}{\partial t}(S^t A)(\boldsymbol{u}) = \sum_i R_i(\boldsymbol{\varphi}(\boldsymbol{u}, t)) \frac{\partial A}{\partial u_i}(\boldsymbol{\varphi}(\boldsymbol{u}, t)) = \sum_i R_i(\boldsymbol{u}) \frac{\partial (S^t A)}{\partial u_i}(\boldsymbol{u}) = L S^t A(\boldsymbol{u}),$$

where L, the Liouvillian, is the linear differential operator $L = \sum_i R_i(\boldsymbol{u}) \frac{\partial}{\partial u_i}$. Thus the phase variable $S^t A$ can be calculated in either of two ways: (i) for each $\boldsymbol{u}$ integrate the equations of motion $\frac{d}{dt}\boldsymbol{\varphi}(\boldsymbol{u}, t) = \boldsymbol{R}(\boldsymbol{\varphi}(\boldsymbol{u}, t))$ with initial condition $\boldsymbol{\varphi}(\boldsymbol{u}, 0) = \boldsymbol{u}$ up to time t and evaluate the phase variable A at the point $\boldsymbol{\varphi}(\boldsymbol{u}, t)$; or (ii) solve the equation

$$\begin{cases} \dfrac{\partial}{\partial t} S^t A = L S^t A \\ S^0 A = A. \end{cases}$$

(In the physics literature S^t is represented symbolically by e^{tL}.)

One can check, from the equivalence of the ways of updating S^tA, that $S^t(AB) = (S^tA)(S^tB)$, that $S^tf(A) = f(S^tA)$, and that S^t commutes with the Liouvillian, $S^tL = LS^t$, where the equality has to be interpreted by considering how each side acts on phase variables.

Suppose that the initial data $\boldsymbol{u}$ are drawn from a probability distribution μ^0; each initial datum gives rise to a solution of equation (2.1) and the measure μ^0 evolves into a measure μ^t at time t. The evolution of μ^t is defined by the condition

$$\int_{\boldsymbol{\Gamma}} B(\boldsymbol{\varphi}(\boldsymbol{u}, t))\, \mu^0(d\boldsymbol{u}) = \int_{\boldsymbol{\Gamma}} B(\boldsymbol{u})\, \mu^t(d\boldsymbol{u})$$

for all sufficiently smooth phase variables B. We assume that the measure μ^0 is invariant under the flow (2.1): $\mu^t = \mu^0$. Given a phase variable B, we denote by $\mathbb{E}[B]$ the expected value of B with respect to the invariant measure μ^0,

$$\mathbb{E}[B] = \int_{\boldsymbol{\Gamma}} B(\boldsymbol{u})\, \mu^0(d\boldsymbol{u}).$$

In this setting, $\boldsymbol{u}$ and $A(\boldsymbol{u})$ can be viewed as random variables.

We now prepare the tools for following a small number of phase variables without calculating the rest. A key quantity is the conditional expectation $\mathbb{E}[B|A]$, where both A and B are phase variables; it satisfies:

1. $\mathbb{E}[B|A]$ is a function of A;

2. $\mathbb{E}[B|A]$ is linear in B:

   $$\mathbb{E}[\alpha B_1 + \beta B_2|A] = \alpha\, \mathbb{E}[B_1|A] + \beta\, \mathbb{E}[B_2|A].$$

3. $\mathbb{E}[B|A]$ is the best approximation of B by a function of A:

   $$\mathbb{E}[|B - \mathbb{E}[B|A]|^2] \leq \mathbb{E}[|B - f(A)|^2] \tag{2.3}$$

   for all functions f. We may regard $\mathcal{P}B = \mathbb{E}[B|A]$ as the orthogonal projection of B on the space of functions of A.

4. For all functions f of A,

$$\mathbb{E}[f(A)(B - \mathbb{E}[B|A])] = 0.$$

5. For all functions f of A,

$$\mathbb{E}[f(A)B|A] = f(A)\mathbb{E}[B|A].$$

See Chung [9].

We now follow the Mori-Zwanzig procedure [8], as modified in [7] and reformulated by us in terms of conditional expectations: we split the time derivative of S^tA into its projection on the span of functions of A plus a complement:

$$\frac{\partial}{\partial t} S^t A = S^t LA = S^t \mathbb{E}[LA|A] + S^t \left(LA - \mathbb{E}[LA|A]\right). \tag{2.4}$$

The first term on the right hand side, $\mathbb{E}[LA|A]$, is the projection of the rate of change of A onto the span of functions of A; we denote it by $\mathfrak{R}(A)$. Thus, the first term is

$$S^t\mathfrak{R}(A) = \mathfrak{R}(S^tA).$$

To understand the second term, consider an evolution operator, $S^t_\perp$, for an arbitrary phase variable, F, which is defined by the following equation:

$$\begin{cases} \dfrac{\partial}{\partial t} S^t_\perp F = LS^t_\perp F - \mathbb{E}[LS^t_\perp F|A] \\ S^0_\perp F = F. \end{cases}, \tag{2.5}$$

Note that

$$\frac{\partial}{\partial t}\mathbb{E}[S^t_\perp F|A] = \mathbb{E}\left[\frac{\partial}{\partial t} S^t_\perp F \middle| A\right] = \mathbb{E}\left[LS^t_\perp F - \mathbb{E}[LS^t_\perp F|A]|A\right] = 0. \tag{2.6}$$

If F is orthogonal to the span of functions of A, then $\mathbb{E}[S^t_\perp F|A] = 0$ for all times t. For this reason, $S^t_\perp$ is referred to as the solution operator of the orthogonal dynamics. We have no general way of solving equation (2.6); a solution in a special case will be described below.

The evolution operators S^t and $S^t_\perp$ satisfy the Dyson formula [8]:

$$S^t B = S^t_\perp B + \int_0^t S^{t-s}\mathbb{E}[LS^s_\perp B|A]\,ds,$$

for all phase variables B, as can be checked by differentiation. In the physics literature this equation is written in the symbolic form

$$e^{tL} = e^{t(I-\mathcal{P})L} + \int_0^t e^{(t-s)L}\mathcal{P}Le^{s(I-\mathcal{P})L}\,ds,$$

which holds when L and $\mathcal{P}$ are linear operators and the exponentials can be properly defined. With the help of the Dyson formula the second term on the right hand side of (2.4) can be written as:

$$S^t_\perp F + \int_0^t S^{t-s}\mathbb{E}[LS^s_\perp F|A]\,ds,$$

where

$$F = LA - \mathbb{E}[LA|A].$$

The phase variable $\mathbb{E}[LS^t_\perp F|A]$ is a function of A which varies in time because $S^t_\perp F$ changes; we denote this function by $K(t,A)$.

Putting all the terms together, we obtain the generalized Langevin equation

$$\frac{\partial}{\partial t}S^t A = \mathfrak{R}(S^t A) + \int_0^t K(s, S^{t-s}A)\,ds + S^t_\perp F. \qquad (2.7)$$

Equation (2.7) is an identity between phase variables which may be vector-valued; it is a starting point for our approximations.

The various terms in equation (2.7) have suggestive interpretations. The first term on the right-hand side is a function only of S^tA and can be interpreted as the self-interaction of the variables S^tA; it is the Markovian contribution to $\frac{\partial}{\partial t}S^tA$. The second term depends on $\boldsymbol{u}$ through the values of S^sA at all times s between 0 and t, and embodies a non-Markovian memory; the kernel $K(t, A)$ is the memory function. Finally, an evaluation of the third term, $S^t_\perp F$, requires a full knowledge of $\boldsymbol{u}$; with our assumptions, this term can be viewed as random, with statistics determined by the distribution of initial data. The expected value of $S^t_\perp F$ conditioned by the initial data vanishes for all t (see (2.6)). Thus, $S^t_\perp F$ is uncorrelated with any function of A; this is a weaker property than statistical independence of $S^t_\perp F$ and A.

3 First-order optimal prediction

We now relate the generalized Langevin equation (2.7) to the first-order optimal prediction schemes of [1, 2, 3, 4]. As before, $\boldsymbol{u} = (u_1, \ldots, u_n)^T$, the equations of motion are

$$\begin{cases} \dfrac{\partial}{\partial t}\boldsymbol{\varphi}(\boldsymbol{u}, t) = \boldsymbol{R}(\boldsymbol{\varphi}(\boldsymbol{u}, t)) \\ \boldsymbol{\varphi}(\boldsymbol{u}, 0) = \boldsymbol{u}, \end{cases}$$

the initial conditions $\boldsymbol{u}$ are drawn from an invariant measure μ^0, and we choose a vector of phase variables, $A = A(\boldsymbol{u}) = (A_1, \ldots, A_m)^T$.

The first order optimal prediction scheme approximates the expectation value of $S^tA(\boldsymbol{u}) = A(\boldsymbol{\varphi}(\boldsymbol{u}, t))$ by a vector-valued function of time, $\boldsymbol{v}(t) = (v_1, \ldots, v_m)^T$ that satisfies

$$\begin{cases} \dfrac{d}{dt}\boldsymbol{v}(t) = \mathfrak{R}(\boldsymbol{v}(t)) \\ \boldsymbol{v}(0) = A(\boldsymbol{u}), \end{cases} \tag{3.1}$$

where as before $\mathfrak{R}(A) = \mathbb{E}[LA|A]$. A comparison between (2.7) and (3.1) shows that first order optimal prediction is obtained from the generalized Langevin equation by dropping the second and third terms; conditions under which this is legitimate are discussed in [1, 2, 3, 4, 5]. Formula (2.3) in the previous section guarantees that no Markovian approximation of S^tA by a system of m equations can be more accurate, in the mean square sense, than first order optimal prediction.

Consider the special case in which we follow the first m components of $\boldsymbol{u}$, that is, $A(\boldsymbol{u}) = P_m\boldsymbol{u}$, $m < n$, where P_m extracts the first m components of $\boldsymbol{u}$: $P_m\boldsymbol{u} = (u_1, \dots, u_m)^T$. Thus, we have $LA(\boldsymbol{u}) = P_m\boldsymbol{R}(\boldsymbol{u})$ and $S^tA(\boldsymbol{u}) = P_m\boldsymbol{\varphi}(\boldsymbol{u}, t)$. In this case the function $\mathfrak{R}(\boldsymbol{v})$ reduces to

$$\mathfrak{R}(P_m\boldsymbol{u}) = \mathbb{E}[P_m\boldsymbol{R}(\boldsymbol{u})|P_m\boldsymbol{u}], \tag{3.2}$$

where, if the measure μ^0 has a probability density $f_0(u_1, \dots, u_n)$, we have by definition

$$\mathbb{E}[\boldsymbol{R}(\boldsymbol{u})|P_m\boldsymbol{u}] = \frac{\int \boldsymbol{R}(u_1, \dots, u_n)\, f_0(u_1, \dots, u_n)\, du_{m+1} \cdots du_n}{\int f_0(u_1, \dots, u_n)\, du_{m+1} \cdots du_n}.$$

Formula (3.1) with $\mathfrak{R}(\boldsymbol{v})$ given by (3.2) can be contrasted with the Galerkin approximation in terms of m variables, which has the form

$$\frac{d}{dt}\boldsymbol{v} = P_m\boldsymbol{R}(v_1, \dots, v_m, 0, \dots, 0),$$

where the argument of $\boldsymbol{R}$ is a vector of size n whose first m components are those of $\boldsymbol{v}$ and the rest are zero.

First-order optimal prediction takes a particularly simple form when equation (2.1) is Hamiltonian. Assume that $\boldsymbol{u} = (q_1, \dots, q_n, p_1, \dots, p_n)^T$, and that equation (2.1) can be written in the form:

$$\begin{aligned} \frac{d}{dt}q_i &= \frac{\partial H}{\partial p_i} \\ \frac{d}{dt}p_i &= -\frac{\partial H}{\partial q_i} \end{aligned}$$

where $H(q, p)$ is the Hamiltonian. Assume that the invariant measure is the canonical measure whose density is

$$f_0(q_1, \dots, q_n; p_1, \dots, p_n) = Z^{-1}e^{-H},$$

where Z is a normalization factor. Let the reduced description be in terms of the $Q = (Q_1, \dots, Q_m)$ and $P = (P_1, \dots, Q_m)$, $m < n$. The optimal prediction equations for the Q_i are:

$$\begin{aligned}\frac{d}{dt}Q_i &= \mathbb{E}\left[\frac{d}{dt}q_i \middle| Q, P\right] \\ &= \frac{\int \frac{\partial H}{\partial p_i} e^{-H}\, dp_{m+1}\cdots dp_n\, dq_{m+1}\cdots dq_n}{\int e^{-H}\, dp_{m+1}\cdots dp_n\, dq_{m+1}\cdots dq_n} \\ &= \frac{\partial}{\partial P_i}\mathcal{H}(Q, P),\end{aligned}$$

where

$$\mathcal{H}(Q, P) = -\log \int e^{-H}\, dp_{m+1}\cdots dp_n\, dq_{m+1}\cdots dq_n$$

is the reduced, or renormalized, Hamiltonian. Similarly,

$$\frac{d}{dt}P_i = \mathbb{E}\left[\frac{d}{dt}p_i \middle| Q, P\right] = -\frac{\partial}{\partial Q_i}\mathcal{H}(Q, P).$$

The reduced Hamiltonian $\mathcal{H}$ is minus the logarithm of the weighted phase space volume constrained by the known values of the Q and P.

Examples of first-order optimal prediction have been presented in [2, 3, 4]. They yields good results for short times and/or m not too small and/or for systems at low temperature. However, in problems that are so severely underresolved that m components of a solution vector describe the solution poorly, first-order optimal prediction does not yield an accurate estimate of the mean solution at high temperature and long times; the subsequent terms in equation (2.7) must be taken into account. In the following section we show that by taking memory into account one can indeed represent a mean solution accurately and in particular observe the irreversible loss of information that occurs in underresolved approximations.

4 Example: a nonlinear Schrödinger equation

We consider the model problem:

$$\imath u_t = -u_{xx} + \frac{1}{4}(3|u|^2 u + u^{*3}),$$

on $[0, 2\pi]$, with periodic boundary conditions (see [2, 3, 4]). Here u^* denotes the complex conjugate of u and subscripts denote differentiation. The equation is of Schrödinger type, and admits the Hamiltonian

$$H = \frac{1}{2}\int_0^{2\pi} \left[|u_x|^2 + \frac{1}{16}(u^4 + 6|u|^4 + (u^*)^4) \right] dx.$$

We use spectral variables; the unknowns are the complex Fourier coefficients $\boldsymbol{u} = \{u_k; k = 0, 1, -1, \dots\}$. We write the Hamiltonian as

$$H = H(\boldsymbol{u}) = H_0 + H_1,$$

where $H_0(\boldsymbol{u})$ is quadratic in $\boldsymbol{u}$,

$$H_0(\boldsymbol{u}) = \pi \sum_k \omega_k \left| u_k \right|^2,$$

with dispersion relation $\omega_k = k^2$, and

$$H_1(\boldsymbol{u}) = \frac{\pi}{16} \sum_{\substack{k_1,k_2\\k_3,k_4}} \left(u_{k_1} u_{k_2} u_{k_3} u_{k_4} + 6 u_{-k_1} u_{-k_2} u^*_{k_3} u^*_{k_4} + u^*_{k_1} u^*_{k_2} u^*_{k_3} u^*_{k_4} \right) \delta_{k_1,-k_2-k_3-k_4}.$$

Define the Poisson brackets:

$$\{A, B\} = \frac{\imath}{\pi} \sum_j \left(\frac{\partial A}{\partial u_j} \frac{\partial B}{\partial u^*_j} - \frac{\partial B}{\partial u_j} \frac{\partial A}{\partial u^*_j} \right).$$

Then:

$$\{u_k, u_{k'}\} = \{u^*_k, u^*_{k'}\} = 0, \qquad \{u_k, u^*_{k'}\} = \frac{\imath}{\pi}\delta_{k,k'}.$$

The evolution of $\boldsymbol{u}$ is then described by Hamilton's equations,

$$\begin{aligned}\frac{d}{dt}u_k &= \{H, u_k\} = R_k(\boldsymbol{u}) \\ &= -\imath\omega_k u_k - \frac{\imath}{4}\sum_{k_1,k_2,k_3}\left(u^*_{k_1}u^*_{k_2} + 3u_{-k_1}u_{-k_2}\right)u^*_{k_3}\,\delta_{k,-k_1-k_2-k_3}.\end{aligned} \tag{4.1}$$

The operator L which governs the evolution of phase variables is given by

$$L = \sum_k\left[R_k(\boldsymbol{u})\frac{\partial}{\partial u_k} + R^*_k(\boldsymbol{u})\frac{\partial}{\partial u^*_k}\right] = L_0 + L_1, \tag{4.2}$$

where

$$L_0 = -\imath\sum_k \omega_k\left(u_k\frac{\partial}{\partial u_k} - u^*_k\frac{\partial}{\partial u^*_k}\right),$$

and

$$\begin{aligned}L_1 = &-\frac{\imath}{4}\sum_{k,k_1,k_2,k_3}\left(u^*_{k_1}u^*_{k_2} + 3u_{-k_1}u_{-k_2}\right)u^*_{k_3}\,\delta_{k,-k_1-k_2-k_3}\frac{\partial}{\partial u_k} \\ &+\frac{\imath}{4}\sum_{k,k_1,k_2,k_3}\left(u_{k_1}u_{k_2} + 3u^*_{-k_1}u^*_{-k_2}\right)u_{k_3}\,\delta_{k,-k_1-k_2-k_3}\frac{\partial}{\partial u^*_k}.\end{aligned}$$

We choose as invariant measure the canonical measure whose density is proportional to:

$$f_0(\boldsymbol{u}) = e^{-H(\boldsymbol{u})/T},$$

where T, the temperature, specifies the variance of the samples $\boldsymbol{u}$.

The Langevin equation (2.7) allows us to derive equations for a phase variable A (i.e., a set of collective variables) that describes large scale properties of the solution. A reasonable choice of collective variables is the set of Fourier components below some cutoff m, i.e, $A = P_m\boldsymbol{u} = (u_{-m}, \ldots, u_m)^T$. Let B be an arbitrary phase variable; the conditional expectation $\mathbb{E}[B|A] = \mathbb{E}[B|P_m\boldsymbol{u}]$ which enters equation (2.7) is in general hard to evaluate except when f_0 is Gaussian. Following [4] we adopt a perturbative approach and perform a power series expansion in powers of H_1, the non-quadratic part of the Hamiltonian; we then average with respect to the Gaussian measure with density proportional to $e^{-H_0/T}$. By Wick's theorem all the conditional moments of $\boldsymbol{u}$ can be expressed as combinations of the conditional means and covariances,

$$\mathbb{E}_0[u_k|P_m\boldsymbol{u}] = \begin{cases} u_k & \text{if } |k| \leq m \\ 0 & \text{otherwise} \end{cases},$$

$$\mathbb{E}_0[u_k u_q^*|P_m\boldsymbol{u}] = \begin{cases} u_k u_q^* & \text{if } |k|, |q| \leq m \\ (\pi\omega_k)^{-1} T\, \delta_{k,q} & \text{if } |k|, |q| > m \\ 0 & \text{otherwise} \end{cases}.$$

(See [2, 3]).

The Langevin equation (2.7) becomes

$$\frac{d}{dt} S^t P_m \boldsymbol{u} = \mathfrak{R}(S^t P_m \boldsymbol{u}) + \int_0^t \boldsymbol{K}\left(s, S^{t-s} P_m \boldsymbol{u}\right)\, ds + S_\perp^t \boldsymbol{F},$$

where

$$\mathfrak{R}(P_m\boldsymbol{u}) = \mathbb{E}[LP_m\boldsymbol{u}|P_m\boldsymbol{u}], \qquad \boldsymbol{F} = LP_m\boldsymbol{u} - \mathbb{E}[LP_m\boldsymbol{u}|P_m\boldsymbol{u}],$$

and

$$\boldsymbol{K}(s, P_m\boldsymbol{u}) = \mathbb{E}[LS_\perp^s \boldsymbol{F}|P_m\boldsymbol{u}]. \tag{4.3}$$

These expressions can be calculated perturbatively, as we now describe.

The Markovian term, already calculated to first order in [4], has components

$$\begin{aligned} \mathfrak{R}_k(P_m\boldsymbol{u}) \approx & -\imath\,(\omega_k + C)\, u_k \\ & - \frac{\imath}{4} \sum_{|k_1|,|k_2|,|k_3| \leq m} \left(u_{k_1}^* u_{k_2}^* + 3 u_{-k_1} u_{-k_2}\right) u_{k_3}^*\, \delta_{k,-k_1-k_2-k_3}, \end{aligned} \tag{4.4}$$

where

$$C = \frac{3T}{2\pi} \sum_{|k|>m} \frac{1}{\omega_k}.$$

The constant C is a frequency shift that, in the present case, is all that distinguishes first-order optimal prediction from a simple truncation of the Fourier expansion (see [4]). This frequency shift is a decreasing function of the number m of resolved modes and decreases like $1/m$.

We now expand the noise $S_\perp^t \boldsymbol{F}$ as we expanded L in (4.2):

$$\begin{aligned} S_\perp^t F_k \sim{}& S_{\perp,0}^t(I-\mathcal{P})L_0 u_k \\ &+ S_{\perp,0}^t(I-\mathcal{P})L_1 u_k + \int_0^t S_{\perp,0}^{t-s}(I-\mathcal{P})L_1 S_{\perp,0}^s(I-\mathcal{P})L_0 u_k, \end{aligned} \tag{4.5}$$

where $S_{\perp,0}^t$ is the solution operator "orthogonal" to the flow induced by L_0; $S_{\perp,0}^t\boldsymbol{F}$ is a solution of

$$\frac{\partial}{\partial t} S_{\perp,0}^t \boldsymbol{F} = L_0 S_{\perp,0}^t \boldsymbol{F} - \mathbb{E}[L_0 S_{\perp,0}^t \boldsymbol{F} | P_m \boldsymbol{u}],$$

$$S_{\perp,0}^0 \boldsymbol{F} = L_0 P_m \boldsymbol{u} - \mathbb{E}[L_0 P_m \boldsymbol{u} | P_m \boldsymbol{u}].$$

Expression (4.5) simplifies considerably if one notes that the subspace of phase variables that depend only on the u_k, $|k| \leq m$, is closed under the action of L_0; as a result $(I-\mathcal{P})L_0 u_k = 0$ for all $|k| \leq m$, so the first and the third terms on the right hand side of (4.5) vanish. A similar argument yields that $(I-\mathcal{P})L_0\mathcal{P} = 0$, from which it follows that $S_{\perp,0}^t(I-\mathcal{P}) = (1-\mathcal{P})S_0^t$, where S_0^t is the evolution operator generated by L_0 which transforms u_k into $u_k\, e^{-\imath\omega_k t}$. Thus, to leading order the noise equals:

$$\begin{aligned} S_\perp^t F_k \sim{}& (I-\mathcal{P})S_0^t L_1 u_k \\ \sim{}& -\frac{\imath}{4} \sum_{k_1,k_2,k_3} u_{k_1}^* u_{k_2}^* u_{k_3}^* e^{\imath(\omega_{k_1}+\omega_{k_2}+\omega_{k_3})t}\, \delta_{k,-k_1-k_2-k_3} \\ &+ \frac{\imath}{4} \sum_{|k_1|,|k_2|,|k_3|\leq m} u_{k_1}^* u_{k_2}^* u_{k_3}^* e^{\imath(\omega_{k_1}+\omega_{k_2}+\omega_{k_3})t}\, \delta_{k,-k_1-k_2-k_3} \\ &- \frac{3\imath}{4} \sum_{k_1,k_2,k_3} u_{k_1} u_{k_2} u_{k_3}^* e^{\imath(\omega_{k_3}-\omega_{k_1}-\omega_{k_2})t}\, \delta_{k+k_3,k_1+k_2} \\ &+ \frac{3\imath}{4} \sum_{|k_1|,|k_2|,|k_3|\leq m} u_{k_1} u_{k_2} u_{k_3}^* e^{\imath(\omega_{k_3}-\omega_{k_1}-\omega_{k_2})t}\, \delta_{k+k_3,k_1+k_2} \\ &+ \imath C u_k e^{-\imath\omega_k t}. \end{aligned} \tag{4.6}$$

Finally we evaluate the memory kernel, (4.3). Recall that $\mathbb{E}[S_\perp^t \boldsymbol{F}|P_m\boldsymbol{u}] = 0$; from equation (4.8) it follows that to the accuracy with which we are calculating $\mathbb{E}[L_0 S_\perp^t \boldsymbol{F}|P_m\boldsymbol{u}] = 0$, and so the leading order term in the memory kernel $\mathbb{E}[L_1 S_\perp^t \boldsymbol{F}|P_m\boldsymbol{u}]$ is quadratic in L_1 and equals

$$
\begin{aligned}
K_k(t, P_m\boldsymbol{u}) &= \kappa_k(t) u_k \\
&+ \sum_{|k_1|,|k_2|,|k_3|\le m} \phi_{k+k_1}(t) e^{\imath k_1^2 t} u_{k_1}^* \left(u_{k_2}^* u_{k_3}^* + u_{-k_2} u_{-k_3}\right) \delta_{k+k_1,-k_2-k_3} \\
&+ \sum_{|k_1|,|k_2|,|k_3|\le m} \psi_{k-k_1}(t) e^{-\imath k_1^2 t} u_{k_1} u_{k_2} u_{k_3}^* \, \delta_{k-k_1,k_2-k_3}, \\
&+ \frac{3}{16} \sum_{\substack{|k_1|,|k_2|\le m \\ |j_1|,|j_2|,|j_3|\le m \\ |k_3|>m}} (u_{j_1} u_{j_2} + 3u_{-j_1}^* u_{-j_2}^*) u_{j_3} u_{k_1} u_{k_2} \delta_{k_3,-j_1-j_2-j_3} \delta_{k+k_3,k_1+k_2} e^{(\omega_{k_3}-\omega_{k_1}-\omega_{k_2})t} \\
&+ \frac{3}{16} \sum_{\substack{|k_2|,|k_3|\le m \\ |j_1|,|j_2|,|j_3|\le m \\ |k_1|>m}} (u_{j_1} u_{j_2} + 3u_{-j_1}^* u_{-j_2}^*) u_{j_3} u_{k_2}^* u_{k_3}^* \delta_{k_1,-j_1-j_2-j_3} \delta_{k,-k_1-k_2-k_3} e^{(\omega_{k_1}+\omega_{k_2}+\omega_{k_3})t} \\
&- \frac{6}{16} \sum_{\substack{|k_2|,|k_3|\le m \\ |j_1|,|j_2|,|j_3|\le m \\ |k_1|>m}} (u_{j_1}^* u_{j_2}^* + 3u_{-j_1} u_{-j_2}) u_{j_3}^* u_{k_2} u_{k_3}^* \delta_{k_1,-j_1-j_2-j_3} \delta_{k+k_3,k_1+k_2} e^{(\omega_{k_3}-\omega_{k_1}-\omega_{k_2})t}
\end{aligned}
\tag{4.7}
$$

where

$$
\begin{aligned}
\kappa_q(t) = \frac{9T^2\imath}{2\pi^2} \sum_{|k_1|,|k_2|>m} \frac{1}{k_1^2}\frac{1}{k_2^2} \Big[&\sin[(q+k_1+k_2)^2 t] \cos(k_1^2 t) \cos(k_2^2 t) \\
&+ \imath \cos[(q+k_1+k_2)^2 t] \sin(k_1^2 t) \sin(k_2^2 t) \Big],
\end{aligned}
\tag{4.8}
$$

$$
\phi_q(t) = \frac{9T\imath}{4\pi} \sum_{|k|>m} \frac{1}{k^2} \sin\left[\left((q+k)^2 + k^2\right) t\right], \tag{4.9}
$$

and

$$
\psi_q(t) = \frac{9T\imath}{2\pi} \sum_{|k|>m} \frac{1}{k^2} \sin\left[\left((q+k)^2 - k^2\right) t\right].
$$

Thus, the memory kernel consists (to leading order in L_1) of a combination of terms that are either linear, cubic, or quintic in the resolved u_k.

To evaluate $\mathbb{E}[S^t P_m \boldsymbol{u}|P_m \boldsymbol{u}]$ we average (2.7) with respect to the invariant measure conditioned by $P_m \boldsymbol{u}$. The noise term drops out. We approximate $\mathbb{E}[\boldsymbol{R}(S^t P_m \boldsymbol{u})|P_m \boldsymbol{u}]$ by $\mathfrak{R}(\boldsymbol{v}(t))$ and $\mathbb{E}[\boldsymbol{K}(s, S^{t-s} P_m \boldsymbol{u})|P_m \boldsymbol{u}]$ by $\boldsymbol{K}(s, \boldsymbol{v}(t-s))$; with this approximation we find

$$\frac{d}{dt}\boldsymbol{v}(t) = \mathfrak{R}(\boldsymbol{v}(t)) + \int_0^t \boldsymbol{K}(s, \boldsymbol{v}(t-s))\, ds. \tag{4.10}$$

We now show that the memory term is capable of reproducing the decay that first order optimal prediction misses. To do so, we apply the scheme (4.10) to the most underresolved problem within its reach, where A consists solely of the mean value u_0 of $\boldsymbol{u}$, i.e., $m = 0$. The goal is to compute the time evolution of u_0 averaged over all functions initially sampled from the invariant measure, having in common only their mean. We approximate $\mathfrak{R}$, $\boldsymbol{K}$, by the expressions (4.4),(4.7). For $m = 0$ and $T = 1$ equation (4.10) for $v_0(t) \approx \mathbb{E}[S^t u_0|u_0]$ is

$$\begin{aligned} \frac{d}{dt}v_0(t) = -\imath\frac{\pi}{2}v_0(t) - \frac{\imath}{4}\left[(v_0^*(t))^2 + 3(v_0(t))^2\right]\, v_0^*(t) + \int_0^t \kappa_0(s) v_0(t-s)\, ds \\ + \int_0^t \phi_0(s) v_0^*(t-s)\left[(v_0^*(t-s))^2 + (v_0(t-s))^2\right]\, ds. \end{aligned} \tag{4.11}$$

One should note the various sources of error in this approximation, in particular the approximate evaluation of the Markovian term, which is not likely to be accurate when $m = 0$, and the use of a perturbation series which is not likely to be accurate for long times.

The memory kernels $\kappa_0(t)$ and $\phi_0(t)$ have infinite support in time and exhibit recurrent behavior. We truncate these kernels at time $t = 0.9$, chosen so as to produce a reasonable decay; this is consistent with our limited objectives. We will show in later work that when the number of collective variables is larger, a truncation of the memory is harmless.

In Figure 1 we compare the true mean of u_0 computed by a Monte-Carlo method, the mean of u_0 as computed by first-order optimal prediction, and the mean of u_0 as computed from equation (4.11) and a truncated kernel K. As expected, and in agreement with the results in [4], first order optimal prediction eventually fails to capture the relaxation of the means towards their equilibrium values. The inclusion of memory is crucial for capturing this relaxation.

5 Discussion

First-order optimal prediction, as presented in earlier publications, loses accuracy in time; it loses accuracy more rapidly when the number of collective variables is small or when the uncertainty in the initial data, as measured by the temperature, is large; we have shown that the loss of accuracy is less severe than in numerical schemes that make no use of information contained in a prior invariant measure.

In the present paper we have shown that the loss of accuracy in time is analogous to the loss of information in irreversible statistical mechanics: The measure conditioned by the partial initial data converges, in an ergodic system, to the invariant measure, which represents thermal equilibrium. First order optimal prediction takes this effect into account only to the extent possible by the limited number of degrees of freedom that it retains. A formalism of Mori-Zwanzig type shows that the decay is represented by a non-Markovian term; an inclusion of this term produces mean results that can be faithful to the true means for longer times even in severely underresolved situations.

The generalized Langevin equation (2.7) shows that the path to higher accuracy in optimal prediction for underresolved problems lies in a more faithful representation of the initial statistics. In the present paper we have included these higher statistics through a Mori-Zwanzig formalism and a

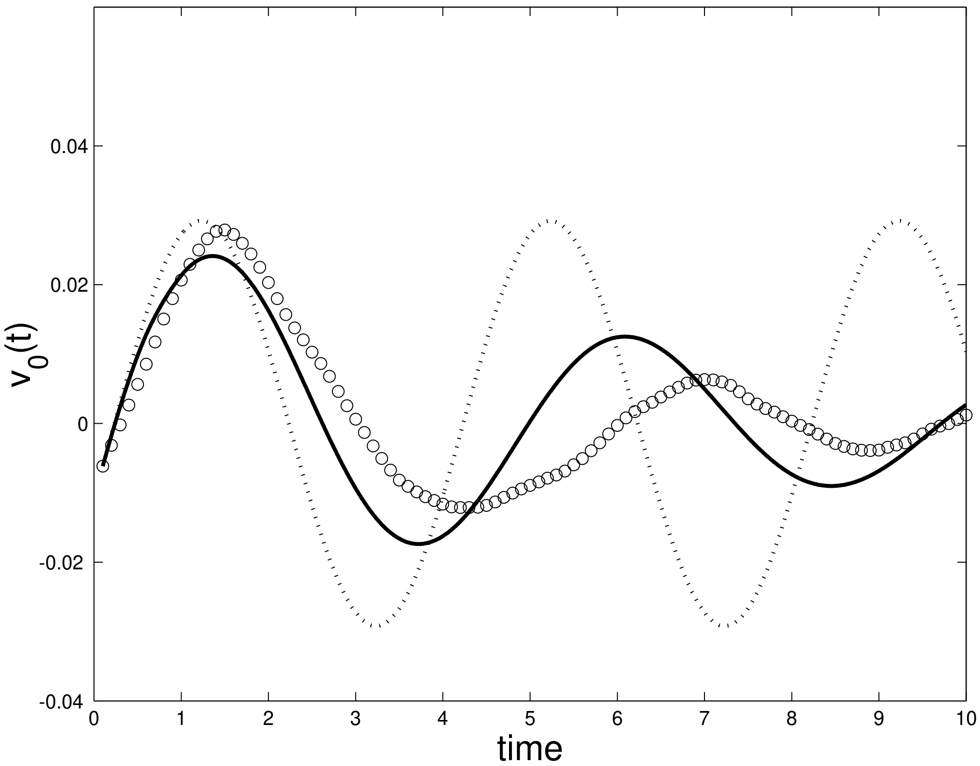

Figure 1: The evolution of the real part of u_0. The circles represent an average over an ensemble of 10^4 solutions which was propagated from a sampled initial ensemble, conditioned only by the value of u_0. The solid line was obtained by integrating the integro-differential equation (4.11) with $\kappa_0(t)$ and $\phi_0(t)$ truncated at $t = 0.9$. Finally, the dotted line was obtained by integrating the first-order optimal prediction equations ($\kappa_0(t) = \phi_0(t) = 0$ in (4.11)).

perturbation scheme, which is too laborious for general use but drives our point home. Practical schemes for higher-order optimal prediction, based on a sampling strategy, will be presented in subsequent work.

Acknowledgments We thank Prof. G.I. Barenblatt, Mr. T. Burin des Roziers, Dr. A. Gottlieb, Dr. A. Kast, and Prof. B. Turkington, for helpful discussions and comments. This work was supported in part by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U.S. Department of Energy, under contract DE–AC03–76–SF00098, and in part by the National Science Foundation under grant DMS94–14631. RK was supported by The Israel Science Foundation founded by The Israel Academy of Sciences and Humanities.

References

[1] Chorin A.J., Kast A.P., Kupferman R., Proc. Nat. Acad. Sci. USA, 95, (1998), pp. 4094–4098.

[2] Chorin A.J., Kast A.P., Kupferman R., Comm. Pure Appl. Math., 52, (1999), pp. 1231–1254.

[3] Chorin A.J., Kast A.P., Kupferman R., Contemp. Math., 238, (1999), pp. 53–75.

[4] Chorin A.J., Kupferman R., and Levy D., Lawrence Berkeley National Laboratory report LBNL-44105, Berkeley, CA, 1999.

[5] Hald O.H., Proc. Nat. Acad. Sci. USA 96 (1999), pp. 4774–4779.

[6] Mori, H., Prog. Th. Phys., 33, (1965), pp. 423–455.

[7] Zwanzig, R., in "Systems Far From Equilibrium", L. Garrido (ed.), Interscience, New York, 1980, pp. 198–221.

[8] Evans, D., Morriss, G., Statistical Mechanics of Non-equilibrium Liquids, Academic Press, NY, 1990.

[9] Chung, K.L., A Course in Probability Theory, Academic, NY (1974).