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# TIME-AVERAGED COARSE VARIABLES FOR MULTI-SCALE DYNAMICS

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**Abstract.** Given an autonomous system of Ordinary Differential Equations without an *a priori* split into slow and fast components, we define a strategy for producing a large class of 'slow' variables (constants of fast motion) in a precise sense. The equation of evolution of any such slow variable is deduced. The strategy is to rewrite our system on an infinite-dimensional "history" Hilbert space $X$ and define our coarse observation as a functional on $X$.

**1. Introduction.** There are three fundamental questions in developing reliable practical models for the deterministic, slow/coarse behavior of a system of autonomous ordinary differential equations (ODE). First, what are the slow variables, if any? Second, can the evolution of such slow variables be written down (as a theory) or be followed by some reliable scheme? Third, is such an evolution closed, i.e. does the set evolve autonomously or, in other words, is a *unique* evolution of the coarse variable set initializable with coarse data?

The first question is important because it is perhaps fair to say that while nature does not provide us with systems (when they can be stated as ODE) with an explicit separation of slow and fast variables, the state-of-the-art today in all of science can reliably predict only the evolution of slow variables once they are known, if that. The second and third questions are of obvious relevance for multiscale modeling.

Despite the vast amount of activity in the field of multiscale modeling in the last decade or so, the first and the third fundamental questions remain largely unanswered, definitely at a rigorous level, for most systems of practical interest. This can be inferred from, e.g., the critical comparative review by an expert in the field (E, [9]) and (Artstein, Gear, Kevrekidis, Slemrod, Titi (AGKST) [5]). Assuming an answer to the first question

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is known, the work of Artstein, Kevrekidis, Slemrod, Titi (AKST) [6] building on earlier work by Artstein and Vigodner (AV) [7] provide rigorous answers to writing down the coarse evolution equation. In AGKST, it is also shown how to utilize the ideas of AKST to approximate the coarse dynamics in a practical manner. However, the existence and explicit knowledge of provably slow variables is a strong requirement in that work. The main result of this paper is to demonstrate a systematic procedure for defining coarse variables that are rigorously shown to be slow in the sense of AKST. The idea is as follows: equilibrium statistical mechanics tells us that under favorable circumstances involving a unique invariant measure for fine dynamics, an infinite time-average is a very good slow variable. Assuming this to be so, it stands to reason that long, but finite, time-averages of phase functions should, in all likelihood, be quite good slow variables. Complications are that

- we are interested in the evolution of the finite time-averages that may be coupled to other slow variables of the system, and equilibrium statistical mechanics provides no clue towards an answer to this question;
- time-averages involve histories and therefore do not directly fit into an averaging framework for ODEs;
- the original system may have a multitude of (unknown) important scales.

We rigorously answer the first two issues in this paper; the third does not end up as a serious impediment since multiscale modeling questions provide great latitude in defining the underlying system that has to be analyzed. We simply chose to completely analyze the response at a certain time-scale provided by physical requirements (e.g. the time-scale of applied loading, considered large in comparison to the typical time-scale of fine dynamics).

Our work makes rigorous a formal scheme proposed and applied to some difficult problems of coarse behavior in [3]. The possibility that AV theory might provide a theoretical basis for the scheme was noted in ([1], [2]), where the averaging problem was explicitly phrased in a form to which AV theory could apply. The applications involved very sudden changes in coarse behavior on a few isolated time intervals, much like what is encountered in relaxation oscillations, so that extrapolating coarse evolution from averaging over fast fine behavior has to be done carefully, if at all. While not directly related to the current discussion, the method used for the applications was based on computing local/overflowing invariant manifolds of an augmented ODE system based on discrete delays of the original fine system. The method is directed towards sequential multiscale modeling and has been applied to many more problems since then, and remains a focus of current research.

This paper is organized as follows: In Section 2, we define a slow-fast system even when the original dynamics does not come equipped with such a split. In Section 3, we provide an alternative compact partial differential equation (PDE)-based formulation for the somewhat clumsy ODE formulation of [2] involving discrete delays, and prove existence of global solutions to the system based on semigroup theory. There are two reasons for providing this formulation:

(1) Unlike the treatment in AKST and AV, here our coarse observable is a functional on an infinite-dimensional 'history' state space. This means that our dynamical

system needs to be posed in an appropriate 'history' state space as well. Nevertheless, with the existence result in hand, in Section 4, we may still apply AKST theory to our slow-fast system and establish that our defined coarse variables are indeed orthogonal measurements (slow variables) of the fast system, in the sense of AKST, and write down their evolution.

(2) As we have mentioned earlier, one option for understanding the evolution of the history-dependent coarse observable is to compute (overflowing) invariant manifolds of the discrete-delay augmented fine ODE system as graphs parametrized by the coarse observable [2]. Depending upon initial data used for the augmenting delay variables, these manifolds can contain trajectories that do not correspond to those of the original system, while containing the latter. While it is certainly possible to require these (overflowing) invariant manifolds of the augmented system to be consistent with only trajectories that arise from the original dynamics, practical experience starting with [3] suggests that if these manifolds were to contain only the latter, they become extremely difficult to compute; it is better to embed the required trajectories in these more general invariant manifolds for the augmented system. Weak solutions to our PDE formulation allow addressing exactly this point in a compact manner.

We end in Section 5 with some speculative remarks on addressing the third fundamental question above.

**2. Definition of the slow-fast system.** We think of an autonomous system of ODEs coupled to applied loads:

$$\begin{aligned} \frac{dz}{dq}(q) &= H(z(q), l(q)), \\ \frac{dl}{dq}(q) &= \frac{1}{\rho} G(z(q), l(q)), \\ z(0) &= z_*, \quad l(0) = l_*. \end{aligned}$$

Here, $(z, l) \in \mathbb{R}^m \times \mathbb{R}^n$, $q$ is the fast time-scale (of MD), and $\rho$ is the time-scale of the applied loading. For example, for linear monotonic strain-controlled loading, it is the applied strain rate; for oscillatory, it would be the fundamental period. Physically, $G$ will typically not depend upon $z$ but we include it here for greater generality. For simplicity of the presentation we will assume $H, G$ to be globally Lipschitz continuous.

We are interested in coarse variables of the type

$$c(q) = \frac{1}{\tau\rho} \int_{q-\tau\rho}^{q} \bar{\Lambda}(z(r))\, dr, \tag{2.1}$$

where $\rho$ is the time-resolution of the measuring apparatus, and $\tau$ is a multiplier of this fundamental period that sets the time-averaging scale for the observables of interest, and $\bar{\Lambda}$ is a state function. For physical reasons, we would like $0 < \tau < 1$.

Introduce the slow time-scale

$$t := \frac{q}{\rho}, \quad \frac{1}{\rho} =: \varepsilon \ll 1.$$

For any given function $f$ of $q$, define the function $\tilde{f}$ of $t$ as follows:

$$\tilde{f}(t) = f(\rho t).$$

Then, on the slow time-scale the system reads

$$\tilde{c}(t) = c(\rho t) = \frac{1}{\tau\rho}\int_{\rho(t-\tau)}^{\rho t} \bar{\Lambda}(z(r))\,dr$$

and the coarse observable reads

$$\tilde{c}(t) = c(\rho t) = \frac{1}{\tau\rho}\int_{\rho(t-\tau)}^{\rho t} \bar{\Lambda}(z(r))\,dr.$$

Introducing the change of variables $p = r/\rho$, we have

$$\tilde{c}(t) = \int_{t-\tau}^{t} \Lambda(\tilde{z}(p))\,dp,$$

where we have used the definition $\Lambda(\cdot) := \bar{\Lambda}(\cdot)\big/\tau$.

We now *drop all overhead tildes* for convenience and focus on the behavior of the following slow-fast system, posed in the slow time-scale:

$$\boxed{\begin{aligned} &\varepsilon\frac{dz}{dt}(t) = H(z(t), l(t)) \\ &\frac{dl}{dt}(t) = G(z(t), l(t)) \\ &c(t) = \int_{t-\tau}^{t} \Lambda(z(p))\,dp. \end{aligned}} \tag{2.2}$$

Recall $(z, l) \in \mathbb{R}^m \times \mathbb{R}^n$ and $\varepsilon$ is a small parameter.

**3. Theory.** As noted in Section 1 and clearly evident from (2.2) our coarse observable $c(t)$ is a functional of the history of $z$ on the interval $[t-\tau, t]$. Thus for consistency our dynamics should be written on a 'history' state space and we do this as follows: set

$$\left.\begin{aligned} x(t,s) &= z(t-s) \\ y(t,s) &= l(t-s) \end{aligned}\right\} \; 0 \le s \le \tau$$

so that the functions $x, y$ will trace out the histories of $z$ and $l$ on intervals $[t-\tau, t]$.

It is easy to see that since $x, y$ are shifts, they satisfy the evolution equations

$$\begin{aligned} \frac{\partial x}{\partial t} &= -\frac{\partial x}{\partial s}, \\ \frac{\partial y}{\partial t} &= -\frac{\partial y}{\partial s}. \end{aligned} \tag{3.1}$$

Hence, if we combine (2.2) and (3.1) we can write the evolution equations as

$$\frac{d}{dt}\begin{pmatrix} x \\ y \\ z \\ l \end{pmatrix} = \begin{pmatrix} -\frac{\partial}{\partial s} & 0 & 0 & 0 \\ 0 & -\frac{\partial}{\partial s} & 0 & 0 \\ 0 & 0 & -I & 0 \\ 0 & 0 & 0 & -I \end{pmatrix}\begin{pmatrix} x \\ y \\ z \\ l \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ z + \frac{H(z,l)}{\varepsilon} \\ l + G(z,l) \end{pmatrix}$$

or

$$\frac{dU}{dt} = AU + F(U),$$

where

$$U = \begin{pmatrix} x \\ y \\ z \\ l \end{pmatrix}, \quad A = \begin{pmatrix} -\frac{\partial}{\partial s} & 0 & 0 & 0 \\ 0 & -\frac{\partial}{\partial s} & 0 & 0 \\ 0 & 0 & -I & 0 \\ 0 & 0 & 0 & -I \end{pmatrix}, \quad F(U) = \begin{pmatrix} 0 \\ 0 \\ z + \frac{H(z,l)}{\varepsilon} \\ l + G(z,l) \end{pmatrix}.$$

Since we are interested in histories, we define the history Hilbert space $X$ as

$$X = \left\{ (x, y, z, l) \in \ L^2(0, \tau; \mathbb{R}^m) \times L^2(0, \tau; \mathbb{R}^n) \times \mathbb{R}^m \times \mathbb{R}^n \right\}$$

with inner product

$$\left( (x, y, z, l), \left( \tilde{x}, \tilde{y}, \tilde{z}, \tilde{l} \right) \right)_X = \int_0^\tau \left( x^T \tilde{x} + y^T \tilde{y} \right) ds + z^T \tilde{z} + l^T \tilde{l},$$

and our operator has domain

$$D(A) = \left\{ (x, y, z, l) \in X : \int_0^\tau \left[ \left( \frac{\partial x}{\partial s} \right)^T \left( \frac{\partial x}{\partial s} \right) + \left( \frac{\partial y}{\partial s} \right)^T \left( \frac{\partial y}{\partial s} \right) \right] ds < \infty, \ x(0) = z, y(0) = l \right\}$$

or

$$D(A) = \left\{ (x, y, z, l) \in H^1(0, \tau; \mathbb{R}^m) \times H^1(0, \tau; \mathbb{R}^n) \times \mathbb{R}^m \times \mathbb{R}^n \text{ and } x(0) = z, y(0) = l \right\}.$$

Let us compute for $U \in D(A)$:

$$\begin{aligned} (AU, U)_X &= -\int_0^\tau \left[ \left( \frac{\partial x}{\partial s} \right)^T \left( \frac{\partial x}{\partial s} \right) + \left( \frac{\partial y}{\partial s} \right)^T \left( \frac{\partial y}{\partial s} \right) \right] ds - z^T z - l^T l \\ &= -\frac{1}{2} \left( x^T(\tau) x(\tau) + y^T(\tau) y(\tau) \right) - \frac{1}{2} \left( z^T z + l^T l \right) \le 0. \end{aligned}$$

In the language of the theory of linear semigroups, the inequality $(AU, U) \le 0$ says that $A$ is 'dissipative'. The Lumer-Phillips Theorem (see, e.g., [10] or [8]) will yield $A$ to be an infinitesimal generator of a linear semigroup of contractions $e^{At}$, i.e.

$$\left\| e^{At} U_0 \right\|_X \le \|U_0\|_X \text{ for all } U_0 \in X,$$

if the range condition

$$AU - \lambda U = V \tag{3.2}$$

can be solved for $U \in D(A)$ $\forall V \in X, \forall \lambda > 0$. Checking the range condition is equivalent to writing $V = \left( \tilde{x}, \tilde{y}, \tilde{z}, \tilde{l} \right)$ and solving

$$\begin{aligned} &-\frac{\partial x}{\partial s} - \lambda x = \tilde{x}, \\ &-\frac{\partial y}{\partial s} - \lambda x = \tilde{y}, \\ &-z \ - \lambda z = \tilde{z}, \\ &-l \ - \lambda l = \tilde{l}, \end{aligned}$$

which yields

$$x(s) = -e^{-\lambda s}\frac{\tilde{z}}{(1+\lambda)} - \int_0^s e^{\lambda(\theta-s)}\tilde{x}(\theta)\, d\theta,$$
$$y(s) = -e^{-\lambda s}\frac{\tilde{l}}{(1+\lambda)} - \int_0^s e^{\lambda(\theta-s)}\tilde{y}(\theta)\, d\theta,$$
$$z = \frac{-\tilde{z}}{(1+\lambda)} \quad ; \quad l = \frac{-\tilde{l}}{(1+\lambda)}$$

and $(x, y, z, l)$ is a solution of (3.2) in $D(A)$. Thus the conditions of the Lumer-Phillips theorem are satisfied.

Note however that for data in $X$ but not in $D(A)$ our formulation allows us to carry the values of $z(t), l(t)$ as distinct entities from their histories $x(t,s) = z(t-s)$, $y(t,s) = l(t-s)$, $0 \le s < \tau$. In particular, the initial conditions for $x, y$, i.e. $x(0,\cdot), y(0,\cdot)$ are merely $L^2(0,\tau : \mathbb{R}^{n \text{ or } m})$ functions and may not have any connection at $s = 0$ with the initial data for $z, l$. On the other hand, for data in $D(A)$, $x(0,0) = z$, $y(0,0) = l$ and we have constructed classical solutions to our evolutionary system.

We may now quote the well-known results of nonlinear evolution equations and recall that our evolutionary system

$$\frac{dU}{dt} = AU + F(U),$$
$$U(0) = U_0 \in X$$

has a unique global mild solution $U(t)$ satisfying

$$U(t) = e^{At}U_0 + \int_0^t e^{A(t-s)}F(U(s))\, ds$$

if $F$ is globally Lipschitz continuous on $X$, and a local solution if $F$ is locally Lipschitz continuous in a neighborhood of $U_0$ ([8], Theorem 1.2, Chapter 6). Moreover, if $F$ is globally Lipschitz, $X$ is reflexive, and $U_0 \in D(A)$, the initial value problem has a unique classical solution ([8], Chapter 6, Theorem 1.7). In our example, $F$ is globally Lipschitz from our assumption that $G, H$ are globally Lipschitz and $X$ is a Hilbert space and hence reflexive.

**4. Application to the slow-fast system.** Let us split $F(U)$ into slow and fast components

$$F_1(U) = \begin{pmatrix} 0 \\ 0 \\ z \\ l + G(z,l) \end{pmatrix} ; \quad F_2(U) = \begin{pmatrix} 0 \\ 0 \\ H(z,l) \\ 0 \end{pmatrix}$$

to write the evolution equation as

$$\frac{dU}{dt} = AU + F_1(U) + \frac{F_2(U)}{\varepsilon}, \tag{4.1}$$

which conveniently denotes our slow-fast decomposition. Following the formulation of AKST we call a continuous functional $v : X \to \mathbb{R}$ a *measurement*. We are interested in measurements which are *constants of motion for the fast flow*, as they produce orthogonal observables (AKST) for which a slow dynamics (not necessarily autonomous) can be written down. Let us define such measurements as *orthogonal measurements*.

Our coarse variable of interest (2.1) motivated the formulation of the problem in a state space involving histories. This formulation along with the time-averaging involved in the definition of the coarse variable immediately provides a *systematic procedure for producing orthogonal measurements*; clearly, any functional on $X$ of the form

$$\begin{aligned} v^*(U(t)) &= \int_0^\tau [\Lambda(x(t,s)) + \Gamma(y(t,s))]\,ds + B(z(t),l(t)) \quad \forall U(t) \in X \\ & \quad \text{with } \nabla_z A \cdot H = 0 \end{aligned} \tag{4.2}$$

will yield a constant of motion of the fast system corresponding to (4.1). Note that the definition has non-null content even for $A = 0$. The only issue is continuity of the functions $\Lambda, \Gamma, A$. Of course, having a sufficient supply of orthogonal measurements is an important ingredient for the practical application of the AKST procedure (cf. AGKST). Define $v(t) = v^*(U(t))$ for $U$ a smooth classical solution corresponding to $U_0 \in D(A)$. If we now compute the value of $\frac{d}{dt}v(t)$ while replacing $x(t,s) = z(t-s)$ and $y(t,s) = l(t-s)$ and setting $\theta = t - s$ we find that

$$v(t) = \int_{t-\tau}^{t} [\Lambda(z(\theta)) + \Gamma(l(\theta))]\,d\theta + B(z(t),l(t)), \tag{4.3}$$

$$\begin{aligned} \frac{dv}{dt}(t) &= [\Lambda(z(t)) + \Gamma(l(t))] - [\Lambda(z(t-\tau)) + \Gamma(l(t-\tau))] \\ &\quad + \nabla_l B(z(t),l(t)) \cdot G(z(t),l(t)). \end{aligned} \tag{4.4}$$

Let $z^{\varepsilon,l,z_0}$ represent solutions of our fast system

$$\varepsilon \frac{dz^{\varepsilon,l,z_0}}{dt} = H\left(z^{\varepsilon,l,z_0}, l\right); \quad z^{\varepsilon,l,z_0}(0) = z_0$$

with $l \in \mathbb{R}^n$ fixed, corresponding to (2.2), and write them in the form

$$z^{\varepsilon,l,z_0}(t) = z^{(0),l,z_0}\left(\frac{t}{\varepsilon}\right) = z^{(0),l,z_0}(q); \quad q = \frac{t}{\varepsilon},$$

where $z^{(0),l,z_0}$ satisfies

$$\frac{dz^{(0),l,z_0}}{dq}(q) = H\left(z^{(0),l,z_0}(q), l\right); \quad z^{(0),l,z_0}(0) = z_0. \tag{4.5}$$

(Notice here that as far as the dynamics of $z^{\varepsilon,l,z_0}$ is concerned, $l$ is frozen since on the fast time-scale $q$ the evolution of $l$ is negligible.) Assume for $0 \le q < \infty$ that $z^{\varepsilon,l,z_0}$ lie in a bounded set of $\mathbb{R}^m$ for each $l$ (with possible $l$ lying in a compact set). Hence, on $[0,T]$ we will have for any continuous function $F$,

$$F\left(z^{\varepsilon,l,z_0}(t)\right) \to \int_{\mathbb{R}^m} F(\lambda)\mu_{t,l,z_0}(\lambda)\,d\lambda \quad \text{weak} * L^\infty[0,T], \tag{4.6}$$

where $\mu_{t,l,z_0}$ is the Young measure generated by the sequence $z^{\varepsilon,l,z_0} \in L^\infty(0,T;\mathbb{R}^m)$. In fact, by results in AKST, $\mu_{t,l,z_0}$ is an invariant measure supported on the $\omega$-limit set of $z^{(0),l,z_0}$.

Motivated by (4.3), let us define the sequence (on $\varepsilon$) of smooth functions $v^{\varepsilon,z_0}$:

$$v^{\varepsilon,z_0}(t) = \int_{t-\tau}^{t} \left[\Lambda\left(z^{\varepsilon,l(\theta),z_0}(\theta)\right) + \Gamma\left(l(\theta)\right)\right] d\theta + B\left(z^{\varepsilon,l(t),z_0}(t), l(t)\right).$$

Then

$$\begin{aligned}\frac{dv^{\varepsilon,z_0}}{dt}(t) &= \left[\Lambda\left(z^{\varepsilon,l(t),z_0}(t)\right) + \Gamma\left(l(t)\right)\right] - \left[\Lambda\left(z^{\varepsilon,l(t-\tau),z_0}(t-\tau)\right) + \Gamma\left(l(t-\tau)\right)\right] \\ &+ \nabla_l B\left(z^{\varepsilon,l(t),z_0}(t), l(t)\right) \cdot G\left(z^{\varepsilon,l(t),z_0}(t), l(t)\right),\end{aligned} \tag{4.7}$$

a time-evolution utilizing the two different sequences $z^{\varepsilon,l(t),z_0}$ and $z^{\varepsilon,l(t-\tau),z_0}$ of fast evolution. Multiplying by any $C^1$ test functions $\varphi$ satisfying $\varphi(0) = \varphi(T) = 0$, after integration by parts we have

$$\begin{aligned}&-\int_0^T \frac{d\varphi}{dt}(t)\, v^{\varepsilon,z_0}(t)\, dt = \\ &\int_0^T \varphi(t) \Big[\Big\{\Lambda\left(z^{\varepsilon,l(t),z_0}(t)\right) + \Gamma\left(l(t)\right)\Big\} - \Big\{\Lambda\left(z^{\varepsilon,l(t-\tau),z_0}(t-\tau)\right) + \Gamma\left(l(t-\tau)\right)\Big\} \\ &\qquad + \nabla_l B\left(z^{\varepsilon,l(t),z_0}(t), l(t)\right) \cdot G\left(z^{\varepsilon,l(t),z_0}(t), l(t)\right)\Big] dt.\end{aligned}$$

Passing to the limit on a subsequence of $\varepsilon$, we see that (4.6) implies that

$$\begin{aligned}-\int_0^T \frac{d\varphi}{dt}(t)\, \bar{v}^{z_0}(t)\, dt = \int_0^T \varphi(t) \Big[&\int_{\mathbb{R}^m} \Lambda(\lambda)\, \mu_{t,l(t),z_0}(\lambda)\, d\lambda \\ &- \int_{\mathbb{R}^m} \Lambda(\lambda)\, \mu_{t-\tau,l(t-\tau),z_0}(\lambda)\, d\lambda \\ &+ \{\Gamma(l(t)) - \Gamma(l(t-\tau))\} \\ &+ \int_{\mathbb{R}^m} \nabla_l B(\lambda, l(t)) \cdot G(\lambda, l(t))\, \mu_{t,l(t),z_0}(\lambda)\, d\lambda\Big] dt,\end{aligned}$$

where $\bar{v}^{z_0}$ is the weak limit of the sequence $v^{\varepsilon,z_0}$. Thus,

$$\begin{aligned}\frac{d\bar{v}^{z_0}}{dt} = &\int_{\mathbb{R}^m} \Lambda(\lambda)\, \mu_{t,l(t),z_0}(\lambda)\, d\lambda - \int_{\mathbb{R}^m} \Lambda(\lambda)\, \mu_{t-\tau,l(t-\tau),z_0}(\lambda) d\lambda + \left[\Gamma(l(t)) - \Gamma(l(t-\tau))\right] \\ &+ \int_{\mathbb{R}^m} \nabla_l B(\lambda, l(t)) \cdot G(\lambda, l(t)) \mu_{t,l(t),z_0}(\lambda)\, d\lambda\end{aligned} \tag{4.8}$$

is satisfied in the weak sense. Similarly, we also have

$$\frac{dl}{dt}(t) = \int_{\mathbb{R}^m} G(\lambda, l(t))\, \mu_{t,l(t),z_0}(\lambda)\, d\lambda \tag{4.9}$$

(where we abuse notation in calling the limit variable by the same name as the fine variable). Physically, we have considered the limit of the instantaneous evolution of our coarse variable $v^{\varepsilon,z_0}$ and defined a limit slow variable $\bar{v}^{z_0}$ as one whose instantaneous evolution is given by (4.8). It should be noted that had the fast evolution characterized by $\frac{1}{\varepsilon}H$ appeared in (4.7), then the Young measure theory could not have been applied to obtain the limit (4.8). Hence, it is important that the coarse function be defined in terms of an orthogonal measurement.

Thus, *we have defined a straightforward way of generating a large class of slow variables via time-averaging and writing their evolution, even if the original system did not come equipped with such slow variables.*

Furthermore, we can use (4.8) to determine the long-term dynamics of the slow-fast system (2.2). This is done in the usual way of multi-scale systems (see, e.g., AGKST):

(1) A sampling step to run the fast system (4.5) and approximate the Young measure as an average of $N$ Dirac masses at $N$ values of $z$;
(2) A long slow time-step using (4.8), (4.9). This gives the evolution of the coarse variables on an interval, say $[0, T]$;
(3) A 'lifting' reconstruction step to find fine data that matches $\bar{v}(T), l(T)$;
(4) Repeat.

It is precisely this procedure that gives an efficient way to compute the dynamics of our coarse observables.

**5. Observations on obtaining a closed coarse dynamics.** A given set of slow variables of a system does not necessarily form a closed set, in the sense of Section 1, w.r.t. coarse evolution. This is best appreciated through examples.

Consider the simplest relaxation oscillation problems in 2 variables (one fast and one slow; see, e.g., [4], Example 2.2),

$$\begin{aligned} \frac{dx}{dt} &= y, \\ \varepsilon \frac{dy}{dt} &= -x + y - y^3. \end{aligned}$$

The limiting slow flow is characterized at most instants of time by

$$\begin{aligned} &\frac{d\bar{x}}{dt} = y_{aug}, \\ &g\left(\bar{x}, y_{aug}\right) = -\bar{x} + y_{aug} - y_{aug}^3 = 0, \end{aligned}$$

and we note that there are situations for the limiting flow where, given only the state of the single slow variable ($\bar{x}$), there are two possibilities for its evolution although that slow variable at any given instant of time evolves in a unique way in reality. Thus, data on a predetermined coarse variable set need not result in unique coarse evolution. However, the unique coarse evolution, perhaps in more than one variable but necessarily *slow*, has to be specified as part of physically meaningful practical modeling, or at least has to be a goal of such modeling endeavors. Indeed, in this example, at most instants the evolution of this additional slow variable is given by

$$\frac{dy_{aug}}{dt} = -\frac{g_{\bar{x}}\left(\bar{x}, y_{aug}\right)}{g_{y_{aug}}\left(\bar{x}, y_{aug}\right)} y_{aug}$$

with initial data satisfying $g\left(\bar{x}, y_{aug}\right) = 0$.

Another illuminating example of this issue arises in Sec. 6.1 of AGKST. Indeed, in their so-called lifting step an initial condition for fine evolution has to be determined corresponding to a given coarse state. As recognized there, this determination cannot in general be unique and an ad-hoc "selection was implemented by carrying the values of two of the entries of the sought vector $\bar{U}$ over from the last simulation." While this particular choice allows for good prediction of coarse response (since, in effect, information on actual fine-scale initial conditions is carried along), it is nevertheless clear that a different choice, based solely on the projected values of the slow variables, could very well have led to an incorrect prediction of coarse response.

Thus, for practical applications, it is essential to attempt to resolve this issue, and below we speculate on a possibility in this regard.

It is clear from the theory (and intuitively) that the invariant measure for the fast dynamics at any given $t$ depends upon the fine initial condition and $l(t)$. Under favorable circumstances, it may be expected that the set of invariant measures characterizing the limit of fast motions for fixed values of the slow variables is finite dimensional (the ergodic case being the simplest where there is only one invariant measure). Intuitively, to have a closed slow dynamics, what we would like to do is to get rid of the dependence on fine initial conditions and have a relation such as

$$\mu_{t,l(t),z_0} = \Upsilon\left(\bar{v}\left(t\right), \bar{v}_{aug}\left(t\right), l\left(t\right)\right) \tag{5.1}$$

exist for almost all $t > 0$ for a suitable finite number of components in the array $\bar{v}_{aug}$. The remaining question is that given a system such as (2.2) is there existence and a characterization of a finite-dimensional set of variables such that a function $\Upsilon$ can be defined. Ideally, this finite-dimensional set of further slow variables should come from sampling the history of the $\bar{v}$s with fixed delays, e.g. $\bar{v}^i_{aug}\left(t\right) = \bar{v}\left(t - d_i\right), i = 1$ to $K$, where $d_i$ is a fixed number. In essence, we would like to have the manifold of invariant measures of the fast dynamics of a system be parametrized by a chosen set of slow variables and their history. Success of this program would imply a mathematical explanation for the *emergence of memory dependence* in coarse response of strictly current state-dependent fine-scale evolution of physical systems.

The evolution equation for such $\bar{v}^i_{aug}$ can be written down following (4.8). We define

$$v^{*i}_{aug}\left(U\left(t\right)\right) = \int_0^{\tau*} p^i\left(s\right)\left[\Lambda\left(x\left(t,s\right)\right) + \Gamma\left(y\left(t,s\right)\right)\right]ds + A^i\left(z\left(t\right), l\left(t\right)\right) \quad \forall U\left(t\right) \in X$$
$$\text{with } \nabla_z A^i \cdot H = 0,$$

where $\tau^* = d_K + \tau$ and each $p^i : [0, \tau^*] \to \mathbb{R}$ is a smoothed bump function with compact support in $[d_i, d_i + \tau]$ approximating a unit-height, step function with finite support. Then, again setting $v^i_{aug}\left(t\right) = v^{*i}_{aug}\left(U\left(t\right)\right)$, $x\left(t,s\right) = z\left(t-s\right)$, $y\left(t,s\right) = l\left(t-s\right)$ and setting $\theta = t - s$ we have

$$\begin{aligned} v^i_{aug}\left(t\right) &= \int_{t-\tau*}^{t} p^i\left(t-\theta\right)\left[\Lambda\left(z\left(\theta\right)\right) + \Gamma\left(l\left(\theta\right)\right)\right]d\theta + A^i\left(z\left(t\right), l\left(t\right)\right) \\ \Rightarrow \frac{dv^i_{aug}}{dt}\left(t\right) &= p^i\left(0\right)\left[\Lambda\left(z\left(t\right)\right) + \Gamma\left(l\left(t\right)\right)\right] - p^i\left(\tau^*\right)\left[\Lambda\left(z\left(t-\tau^*\right)\right) + \Gamma\left(l\left(t-\tau^*\right)\right)\right] \\ &\quad + \int_{t-\tau*}^{t} p^{i'}\left(t-\theta\right)\left[\Lambda\left(z\left(\theta\right)\right) + \Gamma\left(l\left(\theta\right)\right)\right]d\theta \\ &\quad + \nabla_l A^i\left(z\left(t\right), l\left(t\right)\right) \cdot G\left(z\left(t\right), l\left(t\right)\right) \end{aligned}$$

(which is effectively the same as (4.3) noting that $p^{i'}$ approximates the distribution $\delta_{d_i} - \delta_{d_i+\tau}$ and that $p^i\left(0\right)$ and $p^i\left(\tau^*\right)$ are zero for all $i$). Then, following the procedure to go from (4.3) to (4.8) and *assuming* (5.1) holds,

$$\frac{d\bar{v}^i_{aug}}{dt}(t) = p^i(0)\left[\int_{\mathbb{R}^m} \Lambda(\lambda)\Upsilon(\bar{v}(t), \bar{v}_{aug}(t), l(t))(\lambda)\, d\lambda + \Gamma(l(t))\right]$$
$$- p^i(\tau^*)\left[\int_{\mathbb{R}^m} \Lambda(\lambda)\Upsilon(\bar{v}(t-\tau^*), \bar{v}_{aug}(t-\tau^*), l(t-\tau^*))(\lambda)\, d\lambda + \Gamma(l(t-\tau^*))\right]$$
$$+ \int_{t-\tau*}^{t} p^{i\prime}(t-\theta)\left[\int_{\mathbb{R}^m} \Lambda(\lambda)\Upsilon(\bar{v}(\theta), \bar{v}_{aug}(\theta), l(\theta))(\lambda)\, d\lambda + \Gamma(l(\theta))\right] d\theta$$
$$+ \int_{\mathbb{R}^m} \nabla_l A^i(\lambda, l(t)) \cdot G(\lambda, l(t))\, \Upsilon(\bar{v}(t), \bar{v}_{aug}(t), l(t))(\lambda)\, d\lambda$$

holds in a weak sense. For the bump functions employed, this is similar to (4.8) shifted to differences between time-instants $t - d_i$ and $t - d_i - \tau$.

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