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Model Reduction via the Karhunen-Loeve Expansion Part I: An Exposition

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Abstract

In formulating mathematical models for dynamical systems, obtaining a high degree of qualitative correctness (i.e. predictive capability) may not be the only objective. The model must be useful for its intended application, and models of reduced complexity are attractive in many cases. In Part I of this paper we provide an exposition of some techniques that are useful in finding models of reduced complexity for dynamical systems involving flows. The material presented here is not new. The techniques we discuss are based on classical theory such as the Karhunen-Loeve expansion and the method of Galerkin, and the more recent concept of "coherent structures". They have been heavily exploited in a wide range of areas in science and engineering. The attempt here is to present this collection of important methods and ideas together, at a high level of detail, in coherent form, and in the context of model reduction for simulation and control. In this manner we lead in to Part II which illustrates their usefulness in model reduction by applying them to some elementary examples of distributed parameter systems which are related to processes found in semiconductor manufacturing.

1 Introduction

Much of the work of an engineer or scientist is that of formulating suitable mathematical models for a particular physical system. For a dynamical system in continuous time, the model is often some system of ordinary differential equations or partial differential equations. For instance, we might describe the motion of a pendulum with the equations of harmonic motion, or fluid flows with the Navier-Stokes equations. When formulating such models, one of the goals is for the model to maximize qualitative correctness in representing the dynamics of the physical system. For many types of physical systems (far too many to be mentioned here) there exist models whose predictive capability has been demonstrated experimentally. For example, if one solves the Navier-Stokes equations given a set of boundary conditions and initial conditions, the solutions provide an extremely reliable mathematical description of the given fluid flow.

However, in many cases, correctly representing the dynamics is not the sole objective in formulating mathematical models for dynamical systems. In particular, the model needs to be useful for its intended application. For example, if a plant model is required in some kind of real-time feedback control scheme then a model that is computationally intensive may be unsuitable for this purpose. As another example consider a computer simulation of a physical process for which we have a reliable model. We may wish to

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sacrifice some of the correctness of the model in order to make the equations easier to solve, or to allow faster computation of the trajectories. In other words, we have a tradeoff between complexity and correctness.

All of this leads to the following problem. Given a model of a dynamical system that is known to correctly represent the system dynamics, how do we formulate a model of reduced complexity which retains as much of the original predictive capability as possible but which is also amenable to the particular application we have in mind? One classical approach to this problem is via the method of principal components, otherwise called the proper orthogonal decomposition or the Karhunen-Loeve expansion. In this paper, we describe the underlying theory behind this approach, and discuss various issues which arise in its use. We then discuss another classical technique, the method of Galerkin, and show how it is used along with the Karhunen-Loeve expansion to provide reduced order models for dynamical systems involving flows.

The material presented here is not new. As stated before, the techniques we describe are based on classical theory. We also discuss some more recent ideas such as "coherent structures" which is often found in the literature regarding turbulence. Each of the concepts and methods exposed upon here have been heavily exploited in a wide range of areas such as turbulence [3, 4, 12, 13, 14], image processing [11], rapid thermal chemical vapor deposition [1], and identification and control of chemical processes [5]. The attempt here is to present this collection of important methods and ideas together, at a high level of detail, in coherent form, and in the context of model reduction for simulation and control. In this manner we lead in to Part II which illustrates their usefulness in model reduction by applying them to some elementary examples of distributed parameter systems which are related to processes found in semiconductor manufacturing.

I was introduced to the topics covered in this paper by my advisors, P.S. Krishnaprasad and R.A. Adomaitis, with whom I have had many fruitful discussions about all of these topics. The main ideas regarding coherent structures and model reduction spring from several papers by Lawrence Sirovich including [12, 15]. Exposition on random processes and the Karhunen-Loeve expansion is based mainly on Wong's treatment in [16]. Discussion of Galerkin's method is standard and generally follows the treatment in [8]. A list of references is provided at the end of this paper.

2 Flows and Stochastic Processes

In order to limit the scope of this paper somewhat, we shall consider dynamical systems for which solutions to the governing equations give a flow, i.e. a function of time and space that describes the evolution of a particular entity. For example, the quantity of interest could be mass, energy, or momentum. One might be modeling a fluid flow in a chamber governed by the Navier-Stokes equations or heat diffusion on a flat plate governed by the diffusion equation.

Some of the theory of stochastic processes is now introduced in order to provide a framework for modeling these flows which lends itself to formulating models of reduced complexity.

2.1 Modeling the Flow

Let $u(t,x)$ denote a flow. Suppose that the flow is defined on a spatial domain $\mathcal{D}$ (e.g. $\mathcal{D} = [0,M] \times [0,N]$; $M, N > 0$, for a flat plate) and on a time interval T (e.g. we choose $T = [0,\infty)$ for the flows in this paper). Observe that once the initial conditions and boundary conditions are given, the flow, i.e. the solution to the governing equations, is a completely deterministic function of time and space. However, in some cases the flow may still exhibit practically unpredictable behavior. For example, if the evolution of the governing equations is strongly dependent upon initial conditions, then relatively small perturbations in the initial conditions might cause relatively significant qualitative effects on the resulting flow. If these perturbations are undetectable by the available sensors then the exact trajectory of the flow becomes unpredictable. One way to model such unpredictability is by regarding the flow as a random (stochastic) process parameterized by time and space. In this manner, we consider an ensemble of realizations of the flow (e.g. each member

of the ensemble is a trajectory corresponding to a particular initial condition), and introduce a probabilistic structure on the ensemble. We shall denote the flow process by

$$\{u_{t,x}\,;\, t \in [0,\infty), x \in \mathcal{D}\}.$$

Thus the flow is viewed as a two parameter family of real-valued random vectors

$$\{u(t,x,\cdot) : \Omega \to \mathbb{R}^k\}_{t\in[0,\infty),x\in\mathcal{D}}.$$

(Here the flow has been assumed to be k-dimensional, e.g. $k = 3$ for the velocity field of a fluid in a chamber.) The sample space Ω can be thought of as the aforementioned ensemble of completely deterministic realizations of the flow. Nature's choice of $\omega \in \Omega$ yields one of the possible realizations,

$$u(\cdot,\cdot,\omega) : [0,\infty) \times \mathcal{D} \to \mathbb{R}^k.$$

We note that there are difficulties involved in formulating a suitable mathematical description of the sample space Ω, associated σ-algebra $\mathcal{A}$, and probability measure $\mathcal{P}$. The task can be accomplished with some hard work, but, since resolution of these issues is not essential for our purposes, we set them aside for now and proceed as follows. Concepts like expectation (ensemble average) which rely on choice of probability space $(\Omega, \mathcal{A}, \mathcal{P})$ shall simply retain their usual meaning, i.e. $E[X] = \int_\Omega X(\omega)\mathcal{P}(d\omega)$, but cannot be computed without making some further assumptions.

In addition, we define the variation from the mean flow as

$$v_{t,x} = u_{t,x} - E[u_{t,x}].$$

Thus $\{v_{t,x}\}$ is a stochastic process with zero mean.

For the sake of simplicity, and without loss of generality, in this paper we consider only one-dimensional ($k = 1$) flow fields, i.e. the flow field is a two parameter family of real-valued random variables

$$\{u(t,x,\cdot) : \Omega \to \mathbb{R}\}_{t\in[0,\infty),x\in\mathcal{D}}$$

where each $\omega \in \Omega$ represents one particular deterministic flow field

$$u(\cdot,\cdot,\omega) : [0,\infty) \times \mathcal{D} \to \mathbb{R}.$$

For example we consider a fluid with velocity field component in the horizontal direction only, or heat diffusion on a long, thin rod.

2.2 Second-Order Processes

In order to proceed we need to make some assumptions regarding the stochastic processes that we use to model the flows. Some definitions and results from the theory of second-order processes are presented here, suitably tailored for our purposes. In particular, we discuss second order processes, correlation functions, stationarity, and continuity as presented in [16].

Definition 2.1 *A* second-order random variable X *is one which satisfies* $E[|X|^2] < \infty$. *A second-order stochastic process* $\{X_t\}$ *is a one-parameter family of second-order random variables.*

Similarly, we can define a two-parameter second-order stochastic process $\{X_{t,x}\}$ to be a two-parameter family of second-order random variables.

We immediately apply this concept to our flow processes by making the following assumption:

Assumption 2.2 *Let the flow* $\{u_{t,x}\}$ *and deviation from the mean flow* $\{v_{t,x}\}$ *be second-order processes.*

This assumption is necessary for the following reason. If $\{X_t\}$ is a second-order process, then we can define the mean, correlation function, and covariance function, respectively, as follows:

$$\begin{aligned} \mu(t) &= E[X_t] \\ \mathcal{R}(t,s) &= E[X_t X_s] \\ R(t,s) &= E[(X_t - \mu(t))(X_s - \mu(s))] \end{aligned}$$

Note that for a process with zero mean, $R(t,s) = \mathcal{R}(t,s)$ and the covariance and correlation functions can be used interchangeably.

Similarly, for the two-parameter second-order process $\{v_{t,x}\}$ we have

$$\begin{aligned} \mu_v(t,x) &= E[v_{t,x}] \\ \mathcal{R}_v(t,x,s,y) &= E[v_{t,x} v_{s,y}] \\ R_v(t,x,s,y) &= E[(v_{t,x} - \mu_v(t,x))(v_{s,y} - \mu_v(s,y))] \end{aligned}$$

These functions in some sense measure the variation of the flow between different points in space and time. However, for our purposes we are more interested in measuring the spatial variation only (i.e. we fix t). To this end, we define the spatial correlation function as

$$\mathcal{R}_v(x,t,y,t) = E[v_{t,x} v_{t,y}].$$

Similar definitions can be made for the spatial covariance function, temporal correlation function, and temporal covariance function. Since $\{v_{t,x}\}$ is a zero mean process we have

$$R_v(t,x,t,y) = \mathcal{R}_v(t,x,t,y).$$

Before proceeding, one more assumption regarding the correlation functions of the flow processes is necessary.

Assumption 2.3 *Let the flows be* time-stationary*, i.e. for any $(t_1, \ldots, t_n)$ the joint distribution of $\{v_{t_1+t_0,x}, v_{t_2+t_0,x}, \ldots, v_{t_n+t_0,x}\}$ does not depend on t_0.*

One of the reasons we make this assumption is that later we shall want to make some assumptions regarding the ergodicity of the flow process and time-stationarity is a necessary prerequisite. Another reason is that we would like the covariance functions to be time independent. However, for this purpose, we only require the assumption that the flows be *wide-sense stationary*, i.e. their covariance functions are a function of only the time difference. This can be written as

$$E[v_{t+r,x} v_{s+r,y}] = E[v_{t,x} v_{s,y}] \quad \forall r \in [0, \infty).$$

Since this weaker assumption is implied by the stronger statement of time-stationarity, the assumption of time-stationarity suffices. With this assumption we can write the spatial correlation function as

$$E[v_{t,x} v_{t,y}] = R_v(x,y)$$

a function independent of time. We call $R_v(x,y)$ the *two-point spatial correlation function* of the process $\{v_{t,x}\}$.

A covariance function satisfies a number of important properties. Two of great importance for our purposes are the following.

Proposition 2.4 *Every covariance function is Hermitian symmetric, i.e. $R(x,y) = \bar{R}(y,x)$. For a real-valued process it is symmetric, i.e. $R(t,s) = R(s,t)$.*

Proposition 2.5 *Every covariance function is nonnegative definite, i.e. for any finite collection $x_1, x_2, \ldots, x_n$ and complex constants $\alpha_1, \alpha_2, \ldots, \alpha_n$ we have $\sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_j \bar{\alpha}_k R(x_j, x_k) \geq 0$. For a real-valued process the constants α_i simply need be real with no conjugation required.*

The concept of continuity for second-order processes will also be useful.

Definition 2.6 *A second-order process $\{X_t\}$ is* continuous in quadratic mean (q.m. continuous) *at t if $E[|X_{t+h} - X_t|^2] \to 0$ as $h \to 0$. If a process is q.m. continuous at every $t \in T$ then it is a q.m. continuous process.*

One important fact regarding q.m. continuous processes that we shall use is

Proposition 2.7 *If $\{X_t\}$ is a second-order q.m. continuous process on an interval T then its covariance function $R(\cdot, \cdot)$ is continuous at every point on the square $T \times T$.*

Once again we apply the result by making an assumption regarding the flow processes.

Assumption 2.8 *Let the flows $\{u_{t,x}\}$ and $\{v_{t,x}\}$ be q.m. continuous in their spatial argument, i.e. $E[|v_{t,x+h} - v_{t,x}|^2] \to 0$ as $h \to 0$.*

Therefore, if the spatial domain $\mathcal{D}$ is bounded (the proposition requires finite intervals) then the two-point spatial correlation function $R_v(x, y)$ for the flow process $\{v_{t,x}\}$ is continuous in its arguments. Boundedness of the spatial domain is satisfied in many problems of interest, for example fluid flows in a chamber or heat diffusion on a finite sheet or rod.

3 Model Reduction

We wish to find models of the flow fields which lend themselves to a reduction in complexity over the partial differential equation models and which reveal the underlying structure of the flow dynamics. We attempt to accomplish this by considering expansions of the form

$$v(t, x) = \sum_n a_n(t) \phi_n(x). \tag{1}$$

The model can then be reduced in complexity (required computations reduced and/or necessary data compressed) by truncating the series at a suitable value of the index or by using related approaches such as Galerkin's numerical method. We show that if such an expansion is possible then the spatial structures of the flow field are revealed in a spectral decomposition of the two-point spatial correlation function of the process. Also, we show that the desired expansion can be found by employing the Karhunen-Loeve theorem. Finally, we discuss the optimality (in some sense) of using the stated approach.

The background material on Hilbert spaces mainly follows the presentations contained in [6, 8, 16]. The material on the Karhunen-Loeve expansion can be found in [2, 10, 16]. The discussion of coherent structures is based mainly on the treatment by Sirovich in [12]. Discussion of various aspects of this subject can also be found in [1, 3, 4, 7, 11, 13, 14, 15].

3.1 Hilbert Spaces and Orthogonal Expansions

A *Hilbert space* $\mathcal{H}$ is a vector space over $\mathbb{R}$ or $\mathbb{C}$ together with an inner product $< \cdot, \cdot >$ which is complete as a metric space. The norm is defined as $\|\phi\| = \sqrt{< \phi, \phi >}$ for $\phi \in \mathcal{H}$ and the metric is defined as $d(\phi, \psi) = \|\phi - \psi\|$ for $\phi, \psi \in \mathcal{H}$. In this paper, we shall restrict ourselves to Hilbert spaces over $\mathbb{R}$.

The concepts of orthogonality and orthonormal sets will be crucial.

Definition 3.1 *A set of vectors Φ in a Hilbert space $\mathcal{H}$ is an* orthonormal *set if any two distinct vectors $\phi_1, \phi_2 \in \Phi$ are* orthogonal*, i.e. $< \phi_1, \phi_2 >= 0$, and in addition, $\|\phi\| = 1$ for each $\phi \in \Phi$.*

Definition 3.2 *An orthonormal set Φ in a Hilbert space $\mathcal{H}$ is* complete *in $\mathcal{H}$ if there exists no vector in $\mathcal{H}$, except the zero vector, which is orthogonal to every vector in Φ.*

Since we will be considering expansions of the form (1), it makes sense to know under which conditions the series will converge and of what nature are the coefficients.

Proposition 3.3 *If $\Phi = \{\phi_1, \phi_2, \ldots\}$ is an orthonormal set in $\mathcal{H}$ then $\forall y \in \mathcal{H}$, the series*

$$\sum_{n=1}^{\infty} < y, \phi_n > \phi_n$$

converges and if

$$y = \sum_n \alpha_n \phi_n$$

then $\alpha_n =< y, \phi_n >$.

We also wish to determine conditions under which every vector in the Hilbert space is guaranteed to have the stated expansion.

Definition 3.4 *A countable orthonormal set $\Phi = \{\phi_1, \phi_2, \ldots\}$ is an* orthonormal basis *for $\mathcal{H}$ if $\forall y \in \mathcal{H}$, $y = \sum_n \alpha_n \phi_n$ for some $\alpha_1, \alpha_2, \ldots \in \mathbb{R}$.*

By the previous result we know that $\alpha_n =< y, \phi_n >$. Each $< y, \phi_n >$ is called a *Fourier coefficient* of $y \in \mathcal{H}$.

Proposition 3.5 *The orthonormal set $\Phi = \{\phi_1, \phi_2, \ldots\}$ is an orthonormal basis for the Hilbert space $\mathcal{H}$ if and only if Φ is complete in $\mathcal{H}$.*

So, if we can find a complete orthonormal set in the Hilbert space, then every element of the Hilbert space can be expanded in terms of the basis vectors and Fourier coefficients. It is logical to now ask under what conditions a Hilbert space will contain such a complete orthonormal set.

Definition 3.6 *A Hilbert space $\mathcal{H}$ is* separable *if $\mathcal{H}$ contains a countable set which is dense in $\mathcal{H}$.*

Proposition 3.7 *A Hilbert space contains an orthonormal basis if and only if it is separable.*

Proposition 3.8 *Every orthonormal set in a separable Hilbert space is countable.*

In summary, we find that those Hilbert spaces that are separable contain a countable, complete, orthonormal set of vectors, i.e. an orthonormal basis for the Hilbert space, in which every vector in the Hilbert space can be expanded. Finally, we note the following result which states that if such an orthonormal basis exists, it is not unique.

Proposition 3.9 *Given a complete orthonormal set of vectors $\{\phi_n\}$, the set $\{\psi_n\}$ where*

$$\psi_n = \sum_m \alpha_{nm} \phi_m$$

for coefficients satisfying

$$\sum_k \alpha_{ik} \alpha_{jk} = \delta_i^j$$

is also a complete orthonormal set of vectors.

Now we present some important examples of Hilbert spaces which we will use in this paper.

1. $\mathbb{C}^n$, ($\mathbb{R}^n$), the space of n-tuples $(x_1, \ldots, x_n)$ of complex (real) numbers for which $\sum_{i=1}^n |x_i|^2 < \infty$, is an n-dimensional Hilbert space.

2. ℓ_2, the space of infinite sequences $(x_1, x_2, \ldots)$ of complex (or real) numbers for which $\sum_{i=1}^\infty |x_i|^2 < \infty$, is an infinite-dimensional Hilbert space.

3. $\mathcal{L}_2(\mathcal{D})$, the space of complex-valued (real-valued) Lebesgue-measurable square-integrable functions on a domain $\mathcal{D}$, i.e. $f \in \mathcal{L}_2(\mathcal{D})$ if $\int_\mathcal{D} |f(x)|^2\, dx < \infty$, is generally an infinite-dimensional Hilbert space. (This is actually a Hilbert space of equivalence classes of functions but we can treat it as a space of functions by identifying functions which are equal almost everywhere.) The inner product on $\mathcal{L}_2$ is given by
$$< f, g >_{\mathcal{L}_2} = \int_\mathcal{D} f(x)\bar{g}(x)\, dx.$$

Before presenting the next example we need the following definition.

Definition 3.10 *A random variable Y is said to be* derived from a linear operation *on a second order process $\{X_t\}$ if either $Y = \sum_{\nu=1}^N \alpha_\nu X_{t_\nu}$ or Y is the q.m. limit of a sequence of such finite linear combinations.*

4. The collection of all such random variables derived from a given process $\{X_t\}$ is denoted $\mathcal{H}_X$. The set $\mathcal{H}_X$ is generally an infinite-dimensional Hilbert space. The inner product on $\mathcal{H}_X$ is given by
$$< Y, Z >_{\mathcal{H}_X} = E[YZ].$$

We are especially concerned with the following property of the above Hilbert spaces.

Fact 3.11 *All of the above Hilbert spaces are separable, i.e. contain a countable orthonormal basis.*

Moreover, we have the following result.

Proposition 3.12 *Any two separable infinite-dimensional Hilbert spaces are isomorphic.*

Actually, we can make the stronger statement that any two separable Hilbert spaces are linearly isometric. Hence, the last three examples are indistinguishable as Hilbert spaces and we can regard each one as ℓ_2 if we wish.

Let us now see how our flow process $\{v_{t,x}\}$ fits into the Hilbert space framework. Due to the assumption of time-stationarity we can consider the time parameter t to be fixed and regard $\{v_{t,x}\}$ as a continuum of random variables parameterized by the spatial variable x. When interpreting the flow in this manner we shall write the flow as $\{v_x(t)\}$.

The Hilbert space $\mathcal{H}_v$ is defined as the collection of random variables derived from linear operations on the second-order process $\{v_x(t)\}$, i.e. $Y(t) \in \mathcal{H}_v$ is a finite linear combination or q.m. limit of finite linear combinations $Y(t) = \sum_{\nu=1}^N \alpha_\nu v_{x_\nu}(t)$. Clearly $v_x(t) \in \mathcal{H}_v$ for each value of the parameter x. The inner product on $\mathcal{H}_v$ is the two-point spatial correlation function
$$< Y(t), Z(t) >= E[Y_{t,x} Z_{t,y}] = R_{YZ}(x, y).$$

By a previous result, the Hilbert space $\mathcal{H}_v$ has an othonormal basis $\{Z_1(t), Z_2(t), \ldots\}$. Therefore we can write the expansion
$$v_x(t) = \sum_n \sigma_n(x) Z_n(t)$$

where $\sigma_n(x) =< v_x(t), Z_n(t) >$ are the Fourier coefficients. Observe that the orthonormal basis consists of time-dependent random variables while the Fourier coefficients are completely deterministic $\mathcal{L}_2$ functions of space.

Another way to look at the problem is to recall the ω-dependence of the continuum of random variables $\{v_x(t)\}$, i.e. $v_x(t,\cdot) : \Omega \to \mathbb{R}$. Hence for each $\omega \in \Omega$ and for each $t \in [0,\infty)$ we get a deterministic function of $x \in \mathcal{D}$, i.e. $v(t,\cdot,\omega) : \mathcal{D} \to \mathbb{R}$. Due to the assumption of q.m. continuity we can conclude that the function $v(t,\cdot,\omega)$ is square integrable in its spatial argument and therefore $v(t,\cdot,\omega) \in \mathcal{L}_2(\mathcal{D})$. (When interpreting the flow in this manner we shall write the flow as $v(t,\cdot)$.)

By a previous result, the Hilbert space $\mathcal{L}_2(\mathcal{D})$ has an orthonormal basis $\{\phi_1, \phi_2, \ldots\}$. Therefore we can write the expansion

$$v(t,x) = \sum_n a_n(t)\phi_n(x)$$

where $a_n(t) =< v(t,\cdot), \phi_n(\cdot) >_{\mathcal{L}_2}$ are the Fourier coefficients. Observe that the orthonormal basis consists of completely deterministic $\mathcal{L}_2$-functions of space while the Fourier coefficients are time-dependent random variables.

Note that since $\mathcal{H}_v$ and $\mathcal{L}_2(\mathcal{D})$ are isomorphic it does not matter which approach is taken. Both approaches result in an expansion of the flow into a sum of products of pure spatial and pure temporal functions where the time-dependent functions represent a continuum of random variables over the parameter t and the spatial functions are completely deterministic $\mathcal{L}_2$-functions.

3.2 Coherent Structures - Decomposing the Spatial Correlation Function

In order to write the desired expansion

$$v(t,x) = \sum_n a_n(t)\phi_n(x)$$

we first must select a set of basis functions for the Hilbert space that contains v. If we take the approach that $v \in \mathcal{L}_2$ then we must select a basis, $\{\phi_n\}$, for $\mathcal{L}_2$. Similarly, if we take the approach that $v \in \mathcal{H}_v$ then we must select a basis, $\{a_n\}$, for $\mathcal{H}_v$. By previous results we know that each of these Hilbert spaces contains an orthonormal basis, and that in fact an infinite number of such orthonormal basis sets exist for both $\mathcal{L}_2$ and $\mathcal{H}_v$. Fortunately, the following result leads us to a particular choice.

Proposition 3.13 *If $\{\phi_n\}$ is a complete orthonormal set of functions in $\mathcal{L}_2(\mathcal{D})$ such that If the flow process is written as the expansion*

$$v(t,x) = \sum_n a_n(t)\phi_n(x) \tag{2}$$

where both of the sets $\{a_n\}$ and $\{\phi_n\}$ are orthonormal, i.e.

$$< a_k, a_l >_{H_v} = E[a_k(t)a_l(t)] = \delta_k^l, \quad \textit{(uncorrelated modes)} \tag{3}$$

and

$$< \phi_k, \phi_l >_{\mathcal{L}_2} = \int_{\mathcal{D}} \phi_k(x)\phi_l(x) = \delta_k^l, \tag{4}$$

then the $\{\phi_n\}$ are found in a spectral decomposition of the two-point spatial correlation function

$$R(x,y) = \sum_n \phi_n(x)\phi_n(y). \tag{5}$$

(In his treatment of this subject, Sirovich requires only that the set $\{a_n\}$ be orthogonal, i.e. $E[a_k(t)a_l(t)] = \lambda_k\delta_k^l$. In this case the spectral decomposition becomes $R(x,y) = \sum_n \lambda_n\phi_n(x)\phi_n(y)$. The only difference is whether or not the weights λ_n are subsumed into the basis functions ϕ_n.) We now have an

attractive candidate for the orthonormal basis to use for our expansion. We choose the particular orthonormal basis for which the Fourier coefficients of the expansion (2) are also orthonormal (if such a basis exists). Thus, our goal now is to show that this particular orthonormal basis does exist, and to find a practical method for its construction.

The functions $\{\phi_n\}$ in the spectral decomposition of the spatial correlation functions shall be called the coherent structures of the flow.

3.3 The Karhunen-Loeve Expansion

The existence of the expansion (2) which satisfies the orthonormality conditions (3) and (4) is guaranteed under certain conditions by the Karhunen-Loeve expansion theorem. Moreover, the Karhunen-Loeve expansion theorem provides us with a method for constructing the orthonormal set of functions $\{\phi_n\}$ and the uncorrelated set of random variables $\{a_n\}$. The proof depends upon the existence of the aforementioned spectral decomposition of the spatial correlation function (5) which is guaranteed under certain conditions by Mercer's theorem. Thus, we state Mercer's theorem, the Karhunen-Loeve expansion theorem, and show that the desired conditions hold.

Theorem 3.14 (Mercer) *Let $k(\cdot,\cdot)$ be a continuous, Hermitian symmetric, nonnegative definite function on $[a,b]\times[a,b]$. If $\{\phi_n\}$, $\{\lambda_n\}$ is a basic system of eigenvectors and eigenvalues of the integral operator with kernel $k(\cdot,\cdot)$ then $\forall s,t\in[a,b]$,*

$$k(s,t)=\sum_{n=1}^{\infty}\lambda_n\phi_n(t)\phi_n(s).$$

The series converges absolutely and uniformly on $[a,b]\times[a,b]$.

Now we state the Karhunen-Loeve expansion theorem which allows us to express the continuum of random variables by a countable number of orthonormal random variables as presented by Wong in [16].

Theorem 3.15 (Karhunen-Loeve Expansion) *Let $\{X_t\,, t\in[a,b]\}$ be a q.m. continuous second-order process with covariance function $R(t,s)$.*

If $\{\phi_n\}$ are the orthonormal eigenfunctions of the integral operator with kernel $R(\cdot,\cdot)$, and $\{\lambda_n\}$ the corresponding eigenvalues , i.e.

$$\int_a^b R(t,s)\phi_n(s)\,ds=\lambda_n\phi_n(t)\qquad\qquad t\in[a,b] \tag{6}$$

then

$$X(t,\omega)=\lim_{N\to\infty}\sum_{n=1}^{N}\sqrt{\lambda_n}\,a_n(\omega)\phi_n(t)\quad \textit{uniformly for}\quad t\in[a,b] \tag{7}$$

where the limit is taken in the q.m. sense and the $\{a_n\}$ satisfy

$$a_n(\omega)=(\sqrt{\lambda_n})^{-1}\int_a^b\phi_n(t)X(\omega,t)\,dt \tag{8}$$

and

$$E[a_m a_n]=\delta_m^n. \tag{9}$$

Conversely, if $X(t,\omega)$ has an expansion of the form (7) with

$$\int_a^b\phi_m(x)\phi_n(x)\,dx=\delta_m^n$$

and

$$E[a_m a_n] = \delta_m^n$$

then $\{\phi_n\}$ *and* $\{\lambda_n\}$ *must be eigenfunctions and eigenvalues respectively of the integral operator with kernel* $R(\cdot,\cdot)$*, i.e. satisfy (6).*

Proof

Suppose that all functions in the set $\{\phi_n\}$ satisfy the integral equation (6) and that the set of random variables $\{a_n\}$ is defined by (8) so that the orthonormality condition (9) holds.

Let $S_N(t) = \sum_{n=1}^{N} \sqrt{\lambda_n} a_n \phi_n(t)$.

In order to show that the expansion (7) holds, we must show that

$$lim_{N\to\infty} \|X_t - S_N(t)\|^2_{\mathcal{H}_X} = lim_{N\to\infty} E[|X_t - S_N(t)|^2] = 0.$$

Observe that

$$E[|X_t - S_N(t)|^2] = E[|X_t|^2] + E[|S_N(t)|^2] - 2E[X_t S_N(t)] \tag{10}$$

and

$$E[|X_t|^2] = R(t,t) \tag{11}$$

Computing the above terms we get,

$$\begin{aligned}
E[|S_N(t)|^2] &= E[\sum_{n=1}^{N} \sqrt{\lambda_n} a_n \phi_n(t) \sum_{m=1}^{N} \sqrt{\lambda_m} a_m \phi_m(t)] \\
&= E[\sum_{n=1}^{N} \sum_{m=1}^{N} \sqrt{\lambda_n} a_n a_m \phi_n(t) \sqrt{\lambda_m} \phi_m(t)] \\
&= \sum_{n=1}^{N} \sum_{m=1}^{N} \sqrt{\lambda_n}\sqrt{\lambda_m} \phi_n(t)\phi_m(t) E[a_n a_m] \\
&= \sum_{n=1}^{N} \sum_{m=1}^{N} \sqrt{\lambda_n}\sqrt{\lambda_m} \phi_n(t)\phi_m(t) \delta_n^m \\
&= \sum_{n=1}^{N} \lambda_n |\phi_n(t)|^2
\end{aligned}$$

$$\begin{aligned}
E[X_t S_N(t)] &= E[X_t \sum_{n=1}^{N} \sqrt{\lambda_n} a_n \phi_n(t)] \\
&= \sum_{n=1}^{N} \sqrt{\lambda_n} E[X_t a_n \phi_n(t)] \\
&= \sum_{n=1}^{N} \sqrt{\lambda_n} \phi_n(t) E[X_t a_n] \\
&= \sum_{n=1}^{N} \sqrt{\lambda_n} \phi_n(t) E[X_t (\sqrt{\lambda_n})^{-1} \int_a^b \phi_n(s) X_s \, ds] \\
&= \sum_{n=1}^{N} \phi_n(t) \int_a^b \phi_n(s) E[X_t X_s] \, ds \\
&= \sum_{n=1}^{N} \phi_n(t) \int_a^b R(t,s) \phi_n(s) \, ds
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{n=1}^{N} \phi_n(t)(\lambda_n \phi_n(t)) \\
&= \sum_{n=1}^{N} \lambda_n |\phi_n(t)|^2
\end{aligned}
$$

Now, we know from previous results that $R(\cdot,\cdot)$ is Hermitian symmetric and nonnegative definite. We also know that since $\{X_t\}$ is q.m. continuous, $R(\cdot,\cdot)$ is continuous on $[a,b]\times[a,b]$. Therefore, application of Mercer's theorem results in $R(t,s)=\sum_{n=1}^{\infty}\lambda_n\phi_n(t)\phi_n(s)$ and consequently

$$
R(t,t) = \sum_{n=1}^{\infty} \lambda_n |\phi_n(t)|^2 \quad \text{uniformly for} t \in [a,b]. \tag{12}
$$

Substituting into (10) we get

$$
\begin{aligned}
E[|X_t - S_N(t)|^2] &= R(t,t) + \sum_{n=1}^{N} \lambda_n |\phi_n(t)|^2 - 2\sum_{n=1}^{N} \lambda_n |\phi_n(t)|^2 &(13)\\
&= R(t,t) - \sum_{n=1}^{N} \lambda_n |\phi_n(t)|^2 &(14)
\end{aligned}
$$

So by (12) we have the desired result $\lim_{N\to\infty} E[|X_t - S_N(t)|^2] = 0$.

Conversely, suppose X_t has the stated expansion. Then,

$$
R(t,s) = E[X_t X_s] = \sum_{n=0}^{\infty} \lambda_n \phi_n(t)\phi_n(s)
$$

Hence,

$$
\begin{aligned}
\int_a^b R(t,s)\phi_n(s)\,ds &= \int_a^b \sum_{m=0}^{\infty} \lambda_m \phi_m(t)\phi_m(s)\phi_n(s)\,ds \\
&= \sum_m \lambda_m \phi_m(t) \int \phi_m(s)\phi_n(s) ds \\
&= \sum_m \lambda_m \phi_m(t)\delta_m^n \\
&= \lambda_n \phi_n(t)
\end{aligned}
$$

■

In order to apply the result to our flow process $\{v_{t,x}\}$, we invoke the previously stated assumption of time-invariance and get the one-parameter process $v_x(t)$ with two-point spatial covariance $R(x,y)$. The flow is then expanded using the Karhunen-Loeve theorem,

$$
v(t,x) = \sum_{n=1}^{\infty} \sqrt{\lambda_n} a_n(t)\phi_n(x) \tag{15}
$$

where the limit is in the qm sense and

$$
a_n(t) = (\sqrt{\lambda_n})^{-1} \int_{\mathcal{D}} \phi_n(x) v(t,x)\,dx \tag{16}
$$

and

$$
E[a_m(t)a_n(t)] = \delta_m^n. \tag{17}
$$

The orthonormal basis functions $\{\phi_n\}$ are found via the integral equation

$$
\int_{\mathcal{D}} R_v(x,y)\phi_n(y)\,dy = \lambda_n \phi_n(x) \qquad\qquad x \in \mathcal{D}. \tag{18}
$$

3.3.1 Expansion of Sampled Data Processes

In many practical applications, the flow process will be measured in discrete time, i.e. the available data is sampled at discrete values of time. Therefore, we now present an analogous Karhunen-Loeve expansion theorem for sampled data processes. The proof of this theorem relies on the spectral theorem for real symmetric matrices which is the finite-dimensional analogue to Mercer's theorem.

Theorem 3.16 *Let $\{X_i(\omega), i \in \natural\}$ be a discrete parameter second-order process with covariance matrix R given by $(R)_{ij} = E[X_i X_j]$.*

If $\{\phi_n\}$ are the orthonormal eigenvectors of the matrix R, i.e. satisfy

$$R\phi_n = \lambda_n \phi_n \quad n = 1, 2, \ldots \tag{19}$$

and $\{\lambda_n\}$ are the corresponding eigenvalues then

$$X_i(\omega) = \lim_{N\to\infty} \sum_{n=1}^{N} \sqrt{\lambda_n}\, b_n(\omega)(\phi_n)_i \tag{20}$$

where the limit is taken in the q.m. sense and the $\{b_n\}$ satisfy

$$b_n(\omega) = (\sqrt{\lambda_n})^{-1} \sum_{i=1}^{\infty} (\phi_n)_i X_i(\omega) \tag{21}$$

and

$$E[b_m b_n] = \delta_m^n \tag{22}$$

Conversely, if $X_i(\omega)$ has an expansion of the form (20) with $\sum_{i=1}^{\infty}(\phi_m)_i(\phi_n)_i = \delta_m^n = E[b_m b_n]$, then $\{\phi_n\}$ and $\{\lambda_n\}$ must be eigenfunctions and eigenvalues respectively of the matrix R, i.e. satisfy (19).

Proof

Let $(S_N)_i = \sum_{n=1}^{N} \sqrt{\lambda_n}(\phi_n)_i b_n$.

$$\begin{aligned} E[|(S_N)_i - X_i|^2] &= E[|(S_n)_i|^2] + E[|X_i|^2] - 2E[X_i(S_N)_i] \\ &= \sum_{n=0}^{N} \lambda_n |(\phi_n)_i|^2 + (R)_{ii} - 2\sum_{n=0}^{N} \lambda_n |(\phi_n)_i|^2 \\ &= (R)_{ii} - \sum_{n=0}^{N} \lambda_n |(\phi_n)_i|^2 \end{aligned}$$

Now, by the spectral theorem for real symmetric matrices, we know that the symmetric positive definite matrix R can be decomposed into the linear combination of dyads of eigenvectors, $R = \sum_{n=1}^{N} \lambda_n \phi_n \phi_n^T$. Hence, $(R)_{ii} = \sum_{n=0}^{N} \lambda_n |(\phi_n)_i|^2$ and we are done.

To prove the converse, suppose X_i has the stated expansion. Then,

$$R = \sum_{n=1}^{N} \lambda_n \phi_n \phi_n^T$$

or

$$(R)_{ij} = \sum_{n=1}^{N} \lambda_n (\phi_n)_i (\phi_n)_j$$

Hence,

$$\begin{aligned} R\phi_m &= \sum_{n=1}^{N} \lambda_n \phi_n \phi_n^T \phi_m \\ &= \sum_{n=1}^{N} \lambda_n \phi_n \delta_m^n \\ &= \lambda_m \phi_m \end{aligned}$$

■

3.4 Optimality of the Karhunen-Loeve Expansion

We wish to demonstrate that the Karhunen-Loeve theorem provides an expansion of the flow which is in some sense optimal for modeling or reconstructing the original solution. Consider the eigenvalues $\{\lambda_n\}$ that correspond to the eigenfunctions $\{\phi_n\}$. These eigenvalues may be interpreted as "the mean energy of the flow $\{v_{t,x}\}$ projected on the ϕ_n-axis in function space." To see this, we define this mean energy projection as $E[| < \phi_n, v > |^2]$. Now,

$$\begin{aligned} E[\,| < \phi_n, v > |^2\,] &= E[\,| \int \phi_n(x) v(t,x)\, dx|^2\,] \\ &= E[\int \phi_n(x) v(t,x)\, dx \int \phi_n(y) v(t,y)\, dy\,] \\ &= E[\int\int \phi_n(x) v(t,x) \phi_n(y) v(t,y)\, dy\, dx\,] \\ &= \int\int \phi_n(x) E[v(t,x)v(t,y)] \phi_n(y)\, dy\, dx \\ &= \int \phi_n(x) \int R(x,y)\phi_n(y)\, dy\, dx \\ &= \int \phi_n(x)(\lambda_n \phi_n(x))\, dx \\ &= \lambda_n \int |\phi_n(x)|^2\, dx \\ &= \lambda_n \end{aligned}$$

We can also gain some insight by invoking the ergodic hypothesis.

Assumption 3.17 *Let the flow processes be ergodic, i.e. time average equals ensemble average for each fixed value of x.*

We can state this mathematically as

$$E[v_{t,x}] = \lim_{T\to\infty} \frac{1}{T} \int_0^T v(t,x)\, dt \quad \forall \text{ fixed } x.$$

By adopting this assumption of ergodicity then we can also interpret the eigenvalues as the average relative time spent by the flow along the ϕ_n-axis, i.e.

$$\lambda_n = \lim_{T\to\infty} \frac{1}{T} \int_0^T | < \phi_n, v > |^2\, dt.$$

Now, assume that the eigenvalues $\{\lambda_n\}$ corresponding to $\{\phi_n\}$ have been ordered so that $\lambda_{i+1} > \lambda_i \; \forall i$. It can be shown [3] that if $\{\psi_n\}$ is some arbitrary set of basis functions in which we expand $v(t,x)$ then

$$\sum_{n=1}^{N} E[| < \phi_n, v > |^2] = \sum_{n=1}^{N} \lambda_n \geq \sum_{n=1}^{N} E[| < \psi_n, v > |^2]$$

for any value of N. Therefore, among all linear decompositions of the flow field, the Karhunen-Loeve expansion is the most efficient in the sense that for a given number of modes N the projection on the subspace used for modeling the flow will on average contain the most energy possible.

There are other approaches to the question of optimality. For example, we may wish to minimize the norm of the difference between the actual solution and the truncated series. Taking this approach we find

$$\|v - \sum_{1}^{N} a_n \phi_n\|^2 = \|v\|^2 + \|\sum_{1}^{N} a_n \phi_n\|^2 - 2 < v, \sum_{1}^{N} a_n \phi_n > .$$

So the original minimization problem amounts to nothing more than maximizing the sum of projections $\sum_1^N < v, \phi_n >$. Thus, this "error minimization" notion of optimality turns out to be equivalent to the previous "data compression" approach.

3.5 Practical Construction of the Coherent Structures

From a practical point of view, difficulties immediately appear in the determination of the eigenfunctions (coherent structures). For computational purposes we must discretize the spatial domain $\mathcal{D}$. Even a relatively coarse discretization of $\mathcal{D}$ results in a very large empirically determined spatial correlation matrix $R(x,y)$. One approach to solving this problem is to sample the empirical flow data at equally spaced time intervals and use a suitable number of these samples in an appropriate manner to perform the required computations. Sirovich refers to this approach as the method of snapshots [12].

3.5.1 Method of Snapshots

Suppose that a simulation or physical experiment is performed which provides us with an empirically determined flow field $v(t,x)$. Let $v^{(n)} = v(n\tau, x)$, τ fixed, represent "snapshots" or samples of the empirically determined flow field, i.e. a sampled data representation of the flow.

Recall that if the ergodic hypothesis is invoked we can write the spatial correlation function as

$$R(x,y) = \lim_{T\to\infty} \frac{1}{T} \int_0^T v(x,t)v(y,t)\, dt. \tag{23}$$

As an approximation, we use the available sampled data to form the empirically determined spatial correlation function

$$\widetilde{R}(x,y) = \lim_{M\to\infty} \frac{1}{M} \sum_{n=1}^{M} v^{(n)}(x)v^{(n)}(y). \tag{24}$$

Since for all practical purposes our empirical data set is limited to a finite number of snapshots, say M samples, we use the approximation

$$\widetilde{R}_M(x,y) = \frac{1}{M} \sum_{n=1}^{M} v^{(n)}(x)v^{(n)}(y). \tag{25}$$

We shall call $\widetilde{R}_M(x,y)$ the empirically determined spatial correlation function. From the K-L theorem we know that the integral operator with kernel $R(x,y)$ is of great importance in computing the basis functions

for an expansion of the flow process. Therefore we examine the integral operator of the approximation $\widetilde{R}_M(x,y)$ as follows.

$$\begin{aligned}\int_{\mathcal{D}} \widetilde{R}_M(x,y)\phi(y)\,dy &= \int_{\mathcal{D}} \frac{1}{M}\sum_{n=1}^{M} v^{(n)}(x)v^{(n)}(y)\phi(y)\,dy &(26)\\ &= \frac{1}{M}\sum_{n=1}^{M} v^{(n)}(x)\int_{\mathcal{D}} v^{(n)}(y)\phi(y)\,dy &(27)\\ &= \sum_{n=1}^{M}\alpha_n v^{(n)}(x) &(28)\end{aligned}$$

Therefore, the span of the integral operator with kernel $\widetilde{R}_M(\cdot,\cdot)$ is at most a M-dimensional subspace of $L_2(\mathcal{D})$. The eigenfunctions of the integral operator with kernel $\widetilde{R}_M(\cdot,\cdot)$ must satisfy

$$\sum_{n=1}^{M}\alpha_n v^{(n)}(x) = \lambda\phi(x). \tag{29}$$

Therefore, the empirical eigenfunctions can be written

$$\phi(x) = \sum_{n=1}^{M} A_n v^{(n)}(x) \tag{30}$$

for some constants $A_1,\ldots,A_M$. We have the remarkable result that the empirical eigenfunctions of the integral operator with kernel $\widetilde{R}_M(\cdot,\cdot)$ are linear combinations of the samples (snapshots) $v^{(1)},\ldots,v^{(M)}$ of the flow.

Recall that our goal is to find a practical method for computing these empirical eigenfunctions, i.e. solving the eigenfunction equation

$$\int_{\mathcal{D}} \widetilde{R}_M(x,y)\phi(y)\,dy = \lambda\phi(x). \tag{31}$$

Substituting (25) for the empirically determined spatial correlation and (30) for the empirical eigenfunctions yields,

$$\begin{aligned}\int_{\mathcal{D}} \frac{1}{M}\sum_{n=1}^{M} v^{(n)}(x)v^{(n)}(y)\sum_{m=1}^{M} A_m v^{(m)}(y)\,dy &= \lambda\sum_{n=1}^{M} A_n v^{(n)}(x)\\ \frac{1}{M}\sum_{n=1}^{M} v^{(n)}(x)\sum_{m=1}^{M} A_m\int_{\mathcal{D}} v^{(n)}(y)v^{(m)}(y)\,dy &= \lambda\sum_{n=1}^{M} A_n v^{(n)}(x)\end{aligned}$$

which we shall write as

$$(CA)^T V = \lambda A^T V$$

where the matrix C is defined by

$$C_{ij} = \frac{1}{M}\int_{\mathcal{D}} v^{(i)}(x)v^{(j)}(x)\,dx,$$

and $A = [A_1,\ldots,A_M]^T$, $V = [v^{(1)}(x),\ldots,v^{(M)}(x)]^T$.

Assumption 3.18 *Let the set of snapshot data samples $\{v^{(1)},\ldots,v^{(M)}\}$ be a linearly independent set.*

With this assumption we guarantee that the Grammian

$$\int_{\mathcal{D}} V(x)V^T(x)\,dx$$

is positive definite and therefore $(CA)^T V(x) = \lambda A^T V(x)$ iff $CA = \lambda A$. This result means that solutions to the equation (31) are equivalent to solutions of

$$CA = \lambda A$$

and we only need to solve the $M \times M$ matrix eigenvector problem. Invertibility of C guarantees M solutions for A. Substituting the constants $\{A_n\}$ which form the eigenvectors A into (30) gives us the desired empirical eigenfunctions.

Note that the quality of the approximation depends upon the choice of the parameter M, the number of data samples.

3.6 Galerkin's Method

In this section, we look at some applications of the theory and model reduction techniques we have discussed. We limit the discussion to consideration of flows governed by systems of PDEs and satisfying given BCs and ICs. We also observe that in this context, the Karhunen-Loeve expansion is strongly related to separation of variables solution methods for transient BVPs. We take the view of Sirovich [12] and MacCluer [8] to recast the BVPs describing the flows into operator format, and see how the ideas presented in this paper are applied to the method of separation of variables and the numerical method of Galerkin.

Suppose we have a system described by the PDEs (in symbolic form)

$$\frac{\partial v}{\partial t} = D(v) \tag{32}$$

with appropriate boundary conditions. We recast this BVP into operator format

$$\dot{v} = Av \tag{33}$$

where A is the implied spatial differential operator belonging naturally to the problem, defined by the spatial partial derivatives and the boundary conditions. Thus, v in (33) may actually be in a vectorial Hilbert space which incorporates the original boundary conditions. Note that time partial differentiation has been replaced by $\dot{v}$, the time rate of change in the energy sense, i.e.

$$\dot{v(t_0)} = \lim_{t \to t_0} \frac{v(t) - v(t_0)}{t - t_0}.$$

The solution $v(t, x)$ to the BVP with IC $v(0, x) = f(x)$ is thought of as a time-varying norm continuous shape with initial shape $f(x)$, i.e. a trajectory in the Hilbert space $\mathcal{L}_2(\mathcal{D})$ whose tangent $\dot{v}$ for each $t > 0$ is Av.

MacCluer [8] presents results regarding conditions on the operator A and its resolvent operator $(\lambda I - A)^{-1}$ for the existence and uniqueness of a separation of variables solution

$$v(t, x) = \sum_{n=1}^{\infty} a_n(t)\phi_n(x)$$

where the ϕ_n are the orthogonal eigenfunctions of the operator A. However, in keeping with the thrust of this paper, we shall employ our stochastic model of the flow v and rely on the theory of empirical eigenfunction expansions. I.e. we expand the flow in terms of the empirically determined eigenfunctions, not the eigenfunctions of the operator A.

Suppose we obtain empirical data via experiment or simulation and generate the empirically determined spatial correlation and empirically determined eigenfunctions and Karhunen-Loeve expansion of the flow

$$v(t,x) = \sum_{n=1}^{\infty} a_n(t)\phi_n(x)$$

One obvious method for implementing this solution is truncation, where the series solution is merely lopped off to an N term series,

$$v(t,x) = \sum_{n=1}^{N} a_n(t)\phi_n(x)$$

One advantage of this approach is complete control over the error, which is orthogonal to the approximate solution. However, so far we have not indicated a method for finding the $a_n(t)$. This motivates the introduction of the *Galerkin method*.

Define the residual (error) as

$$r(t,x) = \frac{\partial v}{\partial t} - D(v).$$

Clearly we wish the residual to be as close to zero as possible. We know that if we can force the residual to be orthogonal to every vector ϕ_n in the orthonormal basis then the residual must be zero since the orthonormal basis is complete in the Hilbert space. More realistically, we can force the residual to be orthogonal to a suitable finite number of basis functions,

$$< r(t,x), \phi_n(x) >= 0 \qquad n = 1, \ldots, N.$$

We have already shown that these projections represent the energy of the residual in the directions of the basis functions. Moreover, by the optimality property of the Karhunen-Loeve expansion, the energy in the residual vanishes in those directions for which the energy in the flow is extremized.

Now let's compute these projections.

$$\begin{aligned} \frac{\partial v}{\partial t} &= \frac{\partial}{\partial t}\sum_{n=1}^{N} a_n(t)\phi_n(x) \\ &= \sum_{n=1}^{N} \dot{a}_n(t)\phi_n(x). \end{aligned}$$

Hence,

$$r(t,x) = \sum_{n=1}^{N} \dot{a}_n(t)\phi_n(x) - D(\sum_{m=1}^{N} a_m(t)\phi_m(x))$$

and

$$\begin{aligned} < r(t,x), \phi_i(x) > &= \int [\sum_{n=1}^{N} \dot{a}_n(t)\phi_n(x) - D(\sum_{m=1}^{N} a_m(t)\phi_m(x))]\phi_i(x)\, dx \\ &= \sum_{n=1}^{N} \dot{a}_n(t) \int \phi_n(x)\phi_i(x) - \int D(\sum_{m=1}^{N} a_m(t)\phi_m(x))\phi_i(x)\, dx \\ &= \dot{a}_i(t) - \int D(\sum_{m=1}^{N} a_m(t)\phi_m(x))\phi_i(x)\, dx \end{aligned}$$

so

$$\dot{a}_i(t) = \int D(\sum_{m=1}^{N} a_m(t)\phi_m(x))\phi_i(x) \; i = 1, \ldots, N.$$

Thus, insisting that the residual be orthogonal to the first N spatial basis functions yields a system of N ordinary differential equations in t. The reduced model is a system of N ordinary differential equations

$$\dot{a} = F(a)$$

where $a = (a_1, \ldots, a_N), F : \mathbb{R}^N \to \mathbb{R}^N$. We can choose N appropriately for our purposes. This approach is known as Galerkin's method.

Remark 3.19 *The trial solution usually has an extra term so that it exactly satisfies the boundary conditions of the problem,*

$$v(t,x) = v_0(t,x) + \sum_{n=1}^{N} a_n(t)\phi_n(x)$$

Remark 3.20 *The initial conditions for the resulting system of ODEs are determined by a second application of the Galerkin approach. We force the residual $I(x) = v(0,x) - v_0(x)$ of the initial conditions to also be orthogonal to the first N basis functions. We obtain a system of N linear equations*

$$a_i(0) =< \phi_i, I(x) > .$$

4 Conclusions

In this paper we have presented techniques that will be useful in finding models of reduced complexity for dynamical systems involving flows. In Part II of this paper [9] we exhibit the usefulness of these methods by applying them to the modeling and simulation of distributed parameter systems such as heat diffusion and other physical phenomena related to semiconductor manufacturing.

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