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LOW-DIMENSIONAL MODELS OF COMPLEX SYSTEMS USING PRINCIPAL INTERACTION PATTERNS

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1. INTRODUCTION

The standard approach to the numerical study of the dynamical behaviour of partial differential equations (PDEs) a priori vested with an infinite number of degrees of freedom consists in their approximation by finite-dimensional dynamical systems. Given the well known fact that the dynamics of PDEs are often confined to attractor sets of relatively low dimension, the construction of minimal dynamical models capturing the principal properties of the complete system is an interesting task. A class of frequently used approximation schemes is formed by the Galerkin methods. The dynamical field is expanded into a finite set of time-independent basisfunctions; projection of the PDE onto these basisfunctions yields a finite-dimensional system of ordinary differential equations (ODEs) for the time evolution of the expansion coefficients. The efficiency of such a dynamical description, i. e. the number of degrees of freedom required to capture the dynamics of the PDE, depends crucially on a proper choice of the basisfunctions. The most traditional approach lies in using eigenfunctions of a suitably chosen linear differential operator, commonly Fourier modes, as basisfunctions. Despite the elegant mathematical framework of these Fourier-Galerkin methods, they often provide a system of equations which is much larger than the true dimensionality of the system since Fourier modes are completely general and not adapted to the particular system under consideration. Hence information on the dynamics of the system has to be incorporated into the choice of the basisfunctions in order to arrive at a dynamical description reflecting more closely the intrinsic dimensionality of the system.

Up to now modes obtained from a Karhunen-Loève (K-L) decomposition (also referred to as Principal Component analysis, Empirical Orthogonal Function analysis or Proper Orthogonal Decomposition) are widely used as basisfunctions in a Galerkin approximation of a PDE in order to arrive at a low-dimensional model. The K-L eigenfunctions allow for an optimal representation of an attractor in high- or even infinite-dimensional phase space by a linear subspace of given dimension in a mean least-squares sense. However, the optimality criterion defining the K-L modes does not refer to the time evolution of the truncated system obtained when projecting the PDE onto these modes. Thus, as has been first pointed out by Hasselmann [1], a methodology taking into account the dynamics of the reduced system in order to define the basic spatial patterns may be the even more efficient (although the considerably more cumbersome) approach when searching for a minimal model. Following the proposition of Hasselmann, a general algorithm for reducing a high-dimensional Galerkin approximation based on Fourier modes to a low-dimensional dynamical system using optimized basisfunctions has been derived and illustrated in the context of a geophysical fluid system by

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Kwasniok [2]. Coherent structures are obtained from a nonlinear minimization procedure based on a dynamical optimality criterion and used as basisfunctions in a dynamical description.

In the present study the methodology outlined in [2] is developed further by deriving an improved optimality criterion for defining the basisfunctions taking into account the time evolution of the reduced system over a finite time rather than only the local map. The novel method is illustrated in the context of the Kuramoto-Sivashinsky equation.

The paper is organized as follows : In section 2 the model system is introduced. Then a spectral model is derived from this system using a standard Fourier-Galerkin procedure. In section 4 a reduced model is formulated. A variational principle for defining an optimal set of basisfunctions in a reduced model is given in section 5. Then the results are presented.

2. THE KURAMOTO-SIVASHINSKY EQUATION

As a model equation to illustrate the novel method we consider the rescaled Kuramoto-Sivashinsky (K-S) equation in one space dimension

$$\frac{\partial u}{\partial t} + 4\frac{\partial^4 u}{\partial x^4} + \alpha\left[\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2\right] = 0 \tag{1}$$

subject to periodic boundary conditions

$$u(x,t) = u(x+2\pi,t) \qquad \forall\, t \tag{2}$$

at $\alpha = 84.25$ where a limit cycle solution is observed. The following scalar product is introduced :

$$[u_1, u_2] = \frac{1}{2\pi}\int_0^{2\pi} \frac{\partial u_1}{\partial x}\frac{\partial u_2}{\partial x}\, dx \tag{3}$$

For a discussion of the choice of the scalar product see [3].

The system reduction is now achieved in two steps : First, the PDE is casted into a finite-dimensional dynamical description using a standard Fourier-Galerkin procedure. Secondly, a variational principle is applied in this finite- but high-dimensional phase space in order to identify a low-dimensional subspace optimally suited for the construction of a reduced model.

3. SPECTRAL BASIS

An appropriate set of basis functions for the problem stated in section 2 is

$$\left\{\frac{\sqrt{2}}{k}\cos kx, \frac{\sqrt{2}}{k}\sin kx; k = 1,\cdots,k_{\max}\right\} = \{f_\mu; \mu = 1,\cdots,N\} \tag{4}$$

with

$$[f_\mu, f_\nu] = \delta_{\mu\nu} \tag{5}$$

The wavenumber zero mode is omitted in order to remove the mean drift of eq.(1) as is usually done. u is expanded into a truncated series

$$u = \sum_{\mu=1}^{N} u_\mu f_\mu \ . \tag{6}$$

Insertion of the expansion of eq.(6) into the K-S equation and projection onto the basisfunctions yields the system of modal equations. Test calculations revealed that a truncated model using the Fourier modes up to wavenumber $k_{\max} = 15$ (30 degrees of freedom) is sufficient to capture the long-term dynamics of the K-S equation monitored by first and second moments as well as Fourier spectra at the selected parameter value $\alpha = 84.25$. The model is integrated in time using a pseudospectral method based on a discrete Fourier transform on a grid consisting of 48 equally spaced mesh points (employing the Fast Fourier Transform algorithm). Given the extreme stiffness and sensitivity to the numerical accuracy of ODE models derived from eq.(1) a variable-order, variable-step Backward Differentiation Formula is used as ODE integrator with the error tolerance set at 10^{-12} per time unit. Fig. 1 illustrates the time evolution of the solution. The system exhibits periodic behaviour; the variability is spatially localized at the edges of the interval (cf. also Fig. 4).

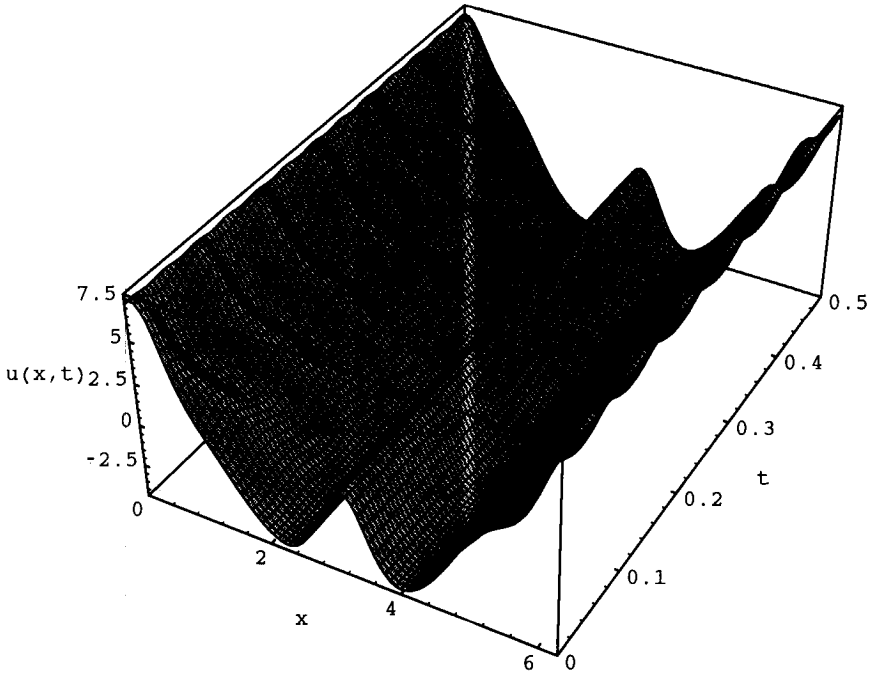

Fig. 1. Galerkin simulation of the K-S equation at $\alpha = 84.25$ using the Fourier modes up to wavenumber 15

4. PRINCIPAL INTERACTION PATTERNS

It is convenient to separate the dynamical field u into the mean state and the deviation from it :

$$u = \langle u \rangle + \hat{u} = \sum_{\mu=1}^{N} (\langle u_\mu \rangle + \hat{u}_\mu)\, f_\mu \tag{7}$$

$\langle \cdot \rangle$ denotes the ensemble average. It is equivalent to the time average assuming ergodicity of the flow. We now consider an L-dimensional subspace spanned by only a limited number of time-independent spatial modes p_i which will be called Principal Interaction Patterns (PIPs). The anomaly field $\hat{u}$ is

expanded into a series of PIPs

$$u = \langle u \rangle + \sum_{i=1}^{L} z_i p_i \ . \tag{8}$$

Without loss of generality the patterns can be assumed to form an orthonormal set [3] :

$$[p_i, p_j] = \delta_{ij} \tag{9}$$

The expansion coefficients are then given by

$$z_i = [p_i, \hat{u}] \ . \tag{10}$$

Projection of the K-S equation onto the PIP-basis yields the system of modal equations

$$\dot{z}_i = \frac{1}{2} \sum_{j,k} a_{ijk} z_j z_k + \sum_j b_{ij} z_j + c_i \tag{11}$$

where the interaction coefficients are given by

$$a_{ijk} = -\alpha \left[p_i, \frac{\partial p_j}{\partial x} \frac{\partial p_k}{\partial x} \right] = a_{ikj} \tag{12}$$

$$b_{ij} = -\left[p_i, 4\frac{\partial^4 p_j}{\partial x^4} + \alpha \frac{\partial^2 p_j}{\partial x^2} + \alpha \frac{\partial \langle u \rangle}{\partial x} \frac{\partial p_j}{\partial x} \right] \tag{13}$$

$$c_i = -\left[p_i, 4\frac{\partial^4 \langle u \rangle}{\partial x^4} + \alpha \frac{\partial^2 \langle u \rangle}{\partial x^2} + \frac{\alpha}{2} \left(\frac{\partial \langle u \rangle}{\partial x} \right)^2 \right] \tag{14}$$

The interaction coefficients can be evaluated numerically using the pseudospectral method.

5. THE VARIATIONAL PRINCIPLE

Consider some initial condition $\hat{u}^0 = \sum_{\mu=1}^{N} \hat{u}_\mu^0 f_\mu$ characterized by the Fourier coefficients $\hat{u}_\mu^0$ at initial time $t = 0$. Let $\hat{u}^\tau = \sum_{\mu=1}^{N} \hat{u}_\mu^\tau f_\mu$ be the state obtained when integrating the Fourier-Galerkin approximation introduced in section 3 forward in time from $t = 0$ to $t = \tau$ with initial condition $\hat{u}^0$. Consider now the projection of the initial condition onto PIP-space $\hat{u}_{\mathrm{PIP}}^0 = \sum_{i=1}^{L} z_i^0 p_i$ with $z_i^0 = [p_i, \hat{u}^0]$. Let $u_{\mathrm{PIP}}^\tau = \sum_{i=1}^{L} z_i^\tau p_i$ be the state obtained when integrating the PIP-model forward in time from $t = 0$ to $t = \tau$ with initial condition $\hat{u}_{\mathrm{PIP}}^0$. Now an error function is introduced which measures the spatially integrated squared error between the state given by the full model and that given by the reduced model temporally averaged over an interval $[0, \tau_{\max}]$ normalized by the spatially integrated variance of the system :

$$J(\hat{u}^0, P; \tau_{\max}) = \frac{\frac{1}{\tau_{\max}} \int_0^{\tau_{\max}} [\hat{u}^\tau - \hat{u}_{\mathrm{PIP}}^\tau, \hat{u}^\tau - \hat{u}_{\mathrm{PIP}}^\tau] \, d\tau}{\sum_{\mu=1}^{N} \left\langle \hat{u}_\mu^2 \right\rangle} \tag{15}$$

Taking the ensemble average over all initial conditions $\hat{u}^0$ on the attractor yields an error function which depends only on the pattern set and the parameter $\tau_{\max}$:

$$\chi = \langle J \rangle \tag{16}$$

The optimal set of patterns is determined by minimizing the error function χ. In practice the ensemble average is replaced by the average over a finite number of initial conditions taken at uncorrelated times from a long time series generated by an integration of the spectral system. The maximum time lag τ_{max} is taken to be 0.02 system units in the present example.

The minimization of χ poses a high-dimensional nonlinear optimization problem (with the $N \cdot L$ elements of P as variables) which has to be solved numerically by iterative techniques. The gradient of χ with respect to the components of P can be calculated efficiently using an adjoint method originating from the theory of optimal control. See [3] for details on the numerical minimization procedure.

6. RESULTS

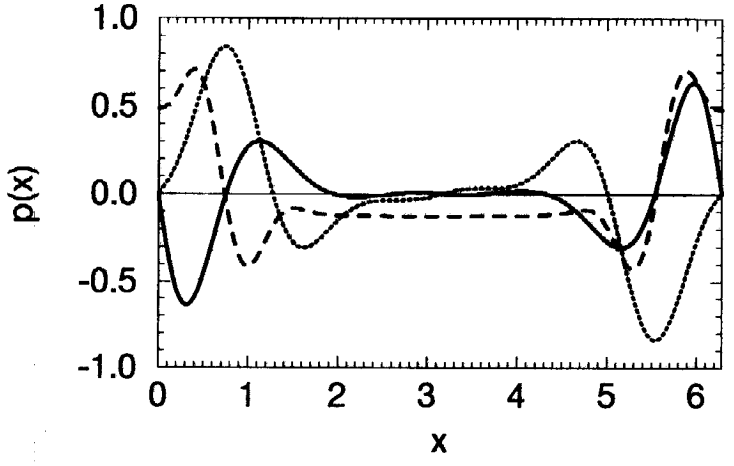

Fig. 2. Spatial structure of the first (solid), second (dotted) and third (dashed) PIP

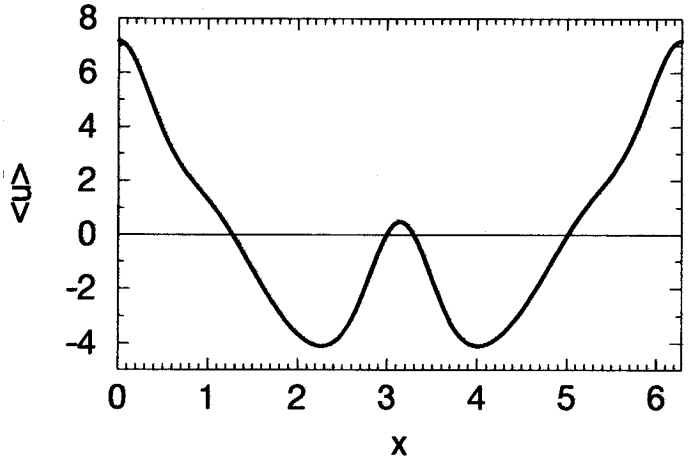

Fig. 3. Mean state obtained from the complete system (solid) and from a simulation with 3 PIPs (dotted)

3 PIPs turned out to be the minimum number of degrees of freedom to capture the dynamics of the K-S equation at the selected value of α. Fig. 2 shows the spatial structure of the patterns extracted from the system. The patterns are ordered by descending mean squared amplitude [3]. Fig. 3 gives the mean state obtained from a long-term integration of the complete system and the reduced system. No difference is visible. The mean state is reproduced perfectly by the PIP-model. Also the variance $\mathrm{Var}(u) = \langle u^2 \rangle - \langle u \rangle^2$ is almost perfectly captured with only 3 degrees of freedom (Fig. 4).

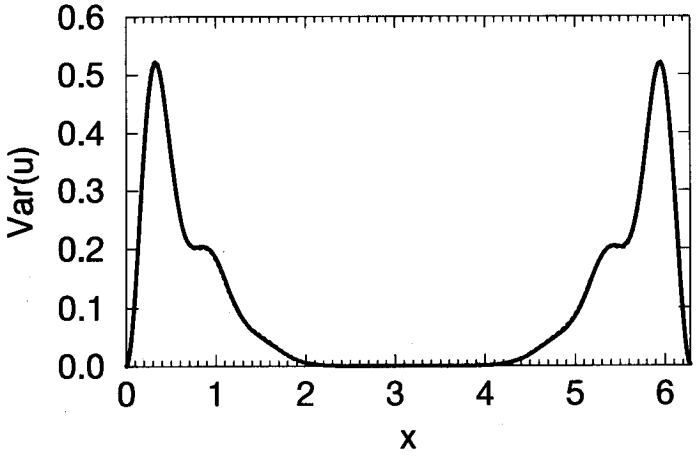

Fig. 4. $\mathrm{Var}(u)$ obtained from the complete system (solid) and from a simulation with 3 PIPs (dotted)

We remark that the technique of Principal Interaction Patterns yields a considerable improvement on more conventional approaches using K-L modes or Sobolev eigenfunctions as basisfunctions.

For a more comprehensive description of this work see [3]. The technique presented here has also been applied to the complex Ginzburg-Landau equation in a chaotic regime [4].

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