Prediction of Complex Flows Part I: Sequential Approximation Of Velocity Fields Using Episodic POD

Dietmar Rempfer
Paritosh Mokhasi

Mechanical, Materials & Aerospace Engineering
Applied Mathematics
Illinois Institute of Technology
Chicago, IL, USA

Industrial Applications of Low-Order Models Based on Proper Orthogonal Decomposition
03/31/2008

Introduction

- Research motivation: Numerical solution of direct and inverse problem of contaminant dispersion

$$\frac{\partial c}{\partial t} + \nabla(\boldsymbol{u}\, c) = \nabla^2(\bar{D}c) + S(x,t).$$

  - Need proper initial and boundary conditions
  - Need 3D velocity field
- Research constraint: Sparse velocity data is available
- Research objective: Develop methods to predict entire 3D velocity fields from sparse data
  - Models that achieve this objective should be (at least)
    - Dynamically consistent
    - Robust to noise and outliers
    - Simple

Focus

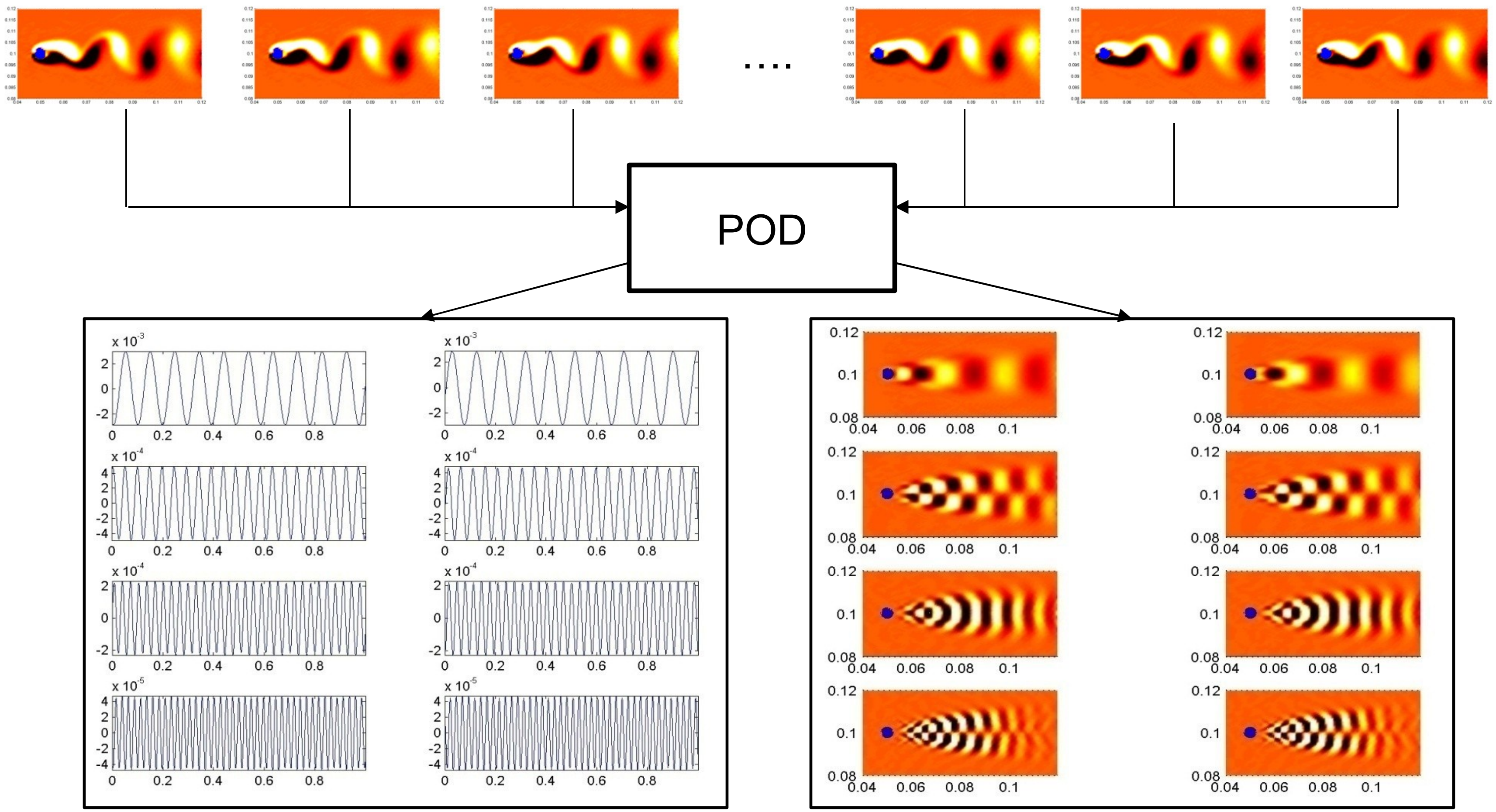
- Development of model that enables approximation of velocity fields at past and future instances in time based on velocity information available at present time step

- Development of *sequential model* that updates previous estimates of velocity fields when new information is provided

Outline

- Proper orthogonal decomposition (POD)
- Episodic POD (Ep-POD)
- Properties of Ep-POD
- Algorithm of model based on Ep-POD
- Validation through examples
  - Flow around 2D cylinder at Re=100
  - 9-D Lorenz model

Proper Orthogonal Decomposition



Ep-POD Model

- A super-snapshot is defined as

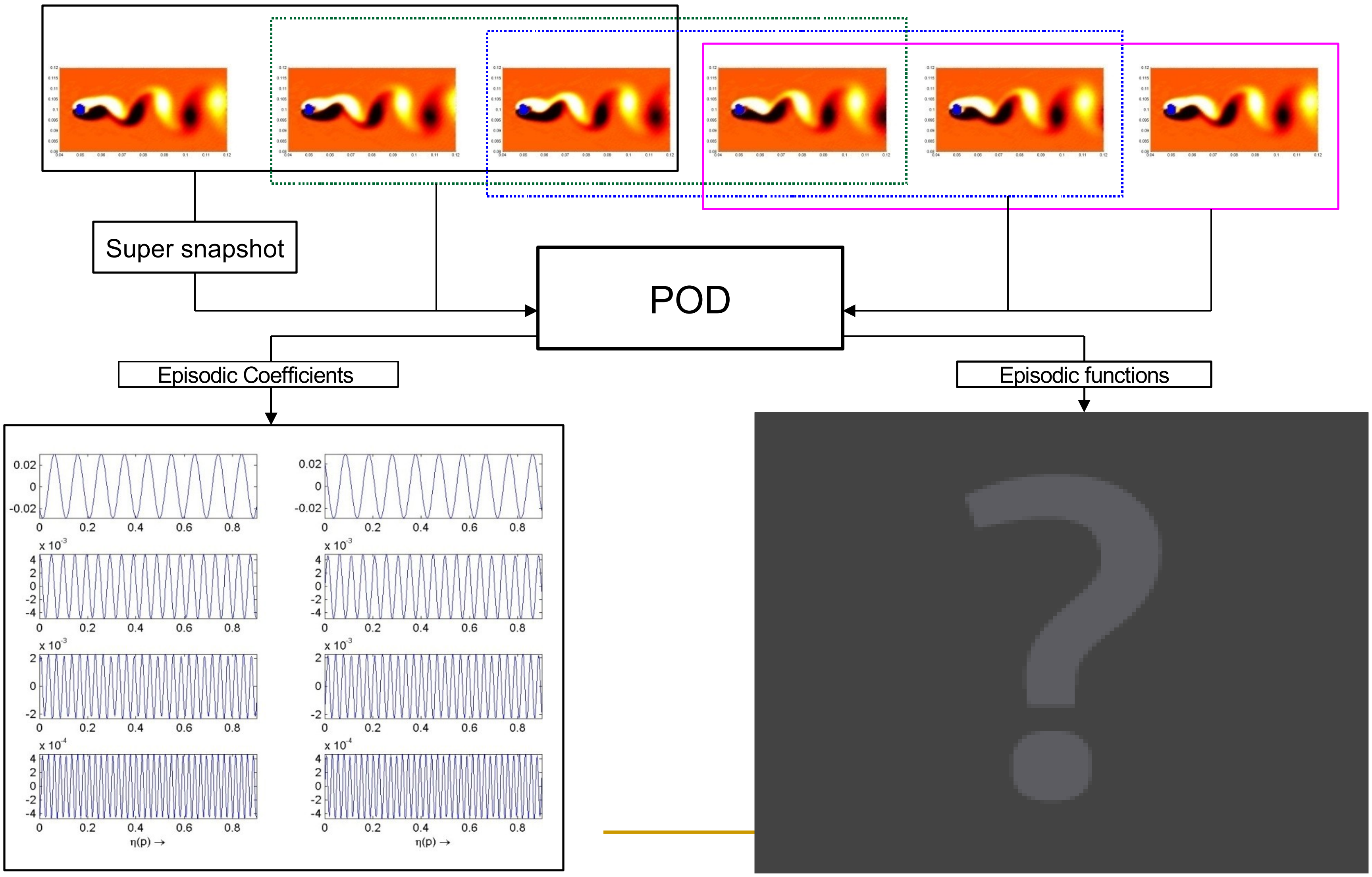
$$\chi_p(x,s) = u(x, t_p + s \cdot (t_{p+T} - t_p)), \quad 0 \leq \ s \ \leq 1.$$

- Ep-POD decomposes the super-snapshot as

$$\chi_p(x,s) = \sum_i \eta_i(p) \Phi_i(x,s)$$

- If the episodic coefficients are known at any given episode, then the spatio-temporal evolution of the velocity field can be approximated within that episode

Episodic Pod



Ep-POD Properties

- Evolution of spatio-temporal basis functions is consistent with definition of Rempfer (1994)

$$\Xi_i(x,t) = \zeta_{2i-1}(t)\psi_{2i-1}(x) + \zeta_{2i}(t)\psi_{2i}(x)$$

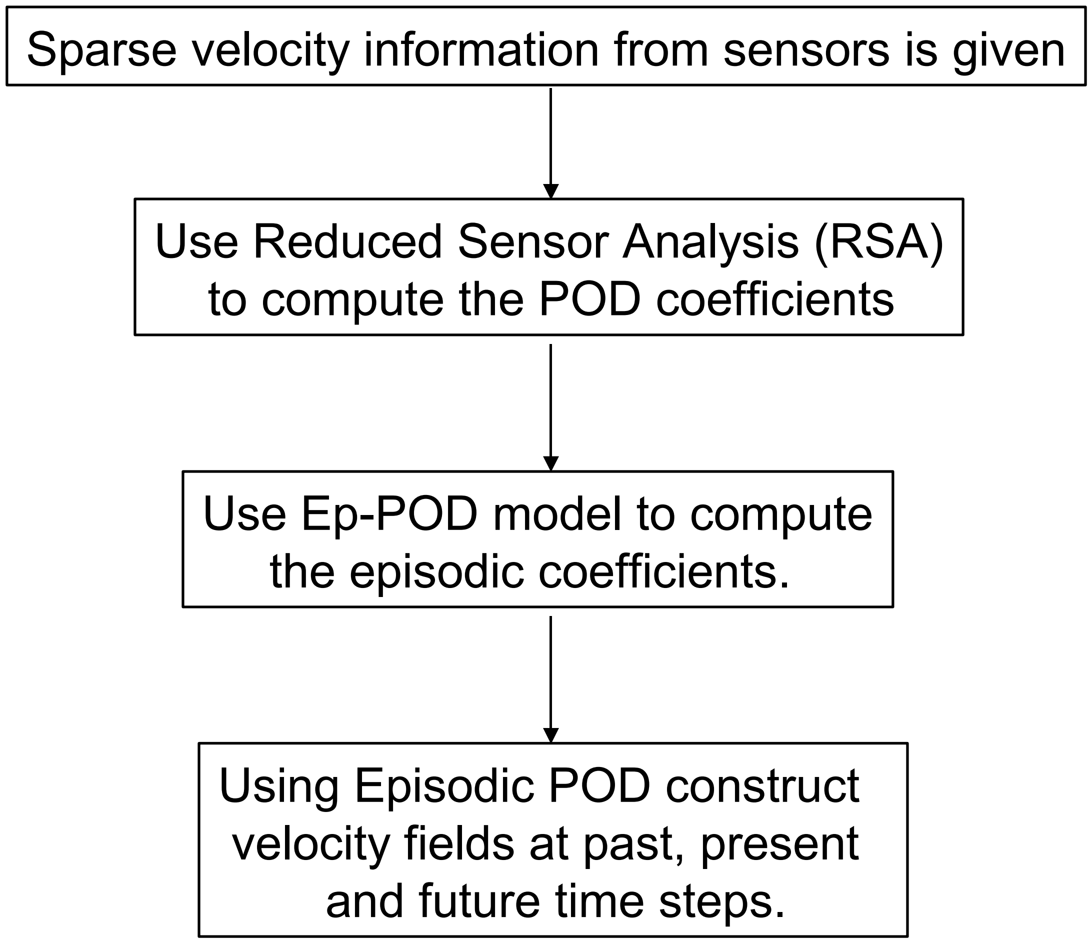
Ep-POD Properties

- Formulation directly leads to a vector-autoregressive (VAR) model for POD coefficients.

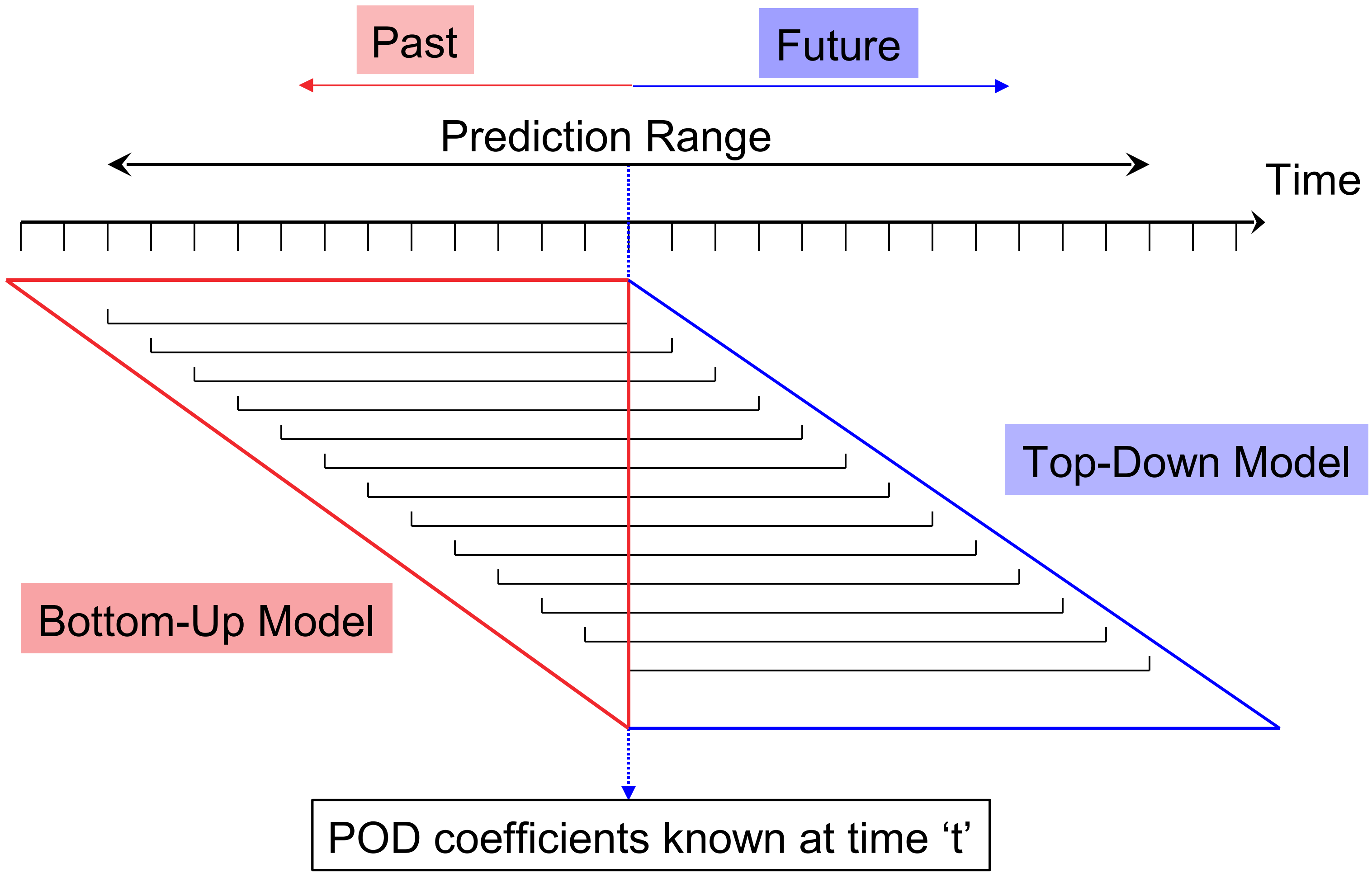
$$\zeta_k(t_{p+T}) = \sum_{m=1} \sum_{n=1}^{n=N-1} \mathcal{C}_{km}(s_n)\,\zeta_m(t_p + s_n(t_{p+T} - t_p))$$

- Models derived from Ep-POD rely on the principle of overlapping snapshots.
  - If there are N snapshots within an episode then there are (N-1) snapshots within the episode that overlap with the previous episode and next episode.
  - For any given episode ‘p’, there exist (2N-1) episodes that share snapshots with the episode ‘p’.

Algorithm for Ep-POD based Model



Algorithms for Ep-POD based Model



Ep-POD based Model

- Bottom-up and top-down models are linear models given by

$$\sum_j \left(\delta_{ij} - \sum_{n=2}^{N} \mathcal{R}_{ij}(n) \right) \eta_j(p) = \sum_k \mathbb{R}_{ik}(s_1)\, \xi_k^p(s_1)$$

- Matrices in model come from principle of overlapping of the spatio-temporal eigenfunctions

Sequential Model

- If information at multiple instances within an episode is available, then Ep-POD based model can be modified to get a sequential model

$$\mathcal{W}_{ij}^{(n)}\,\eta_j^{(n)}(p) = \mathcal{W}_{ij}^{(n-1)}\,\eta_j^{(n-1)}(p) + \mathbb{R}_{ik}(s_\lambda)\,\xi_k^p(s_\lambda),$$

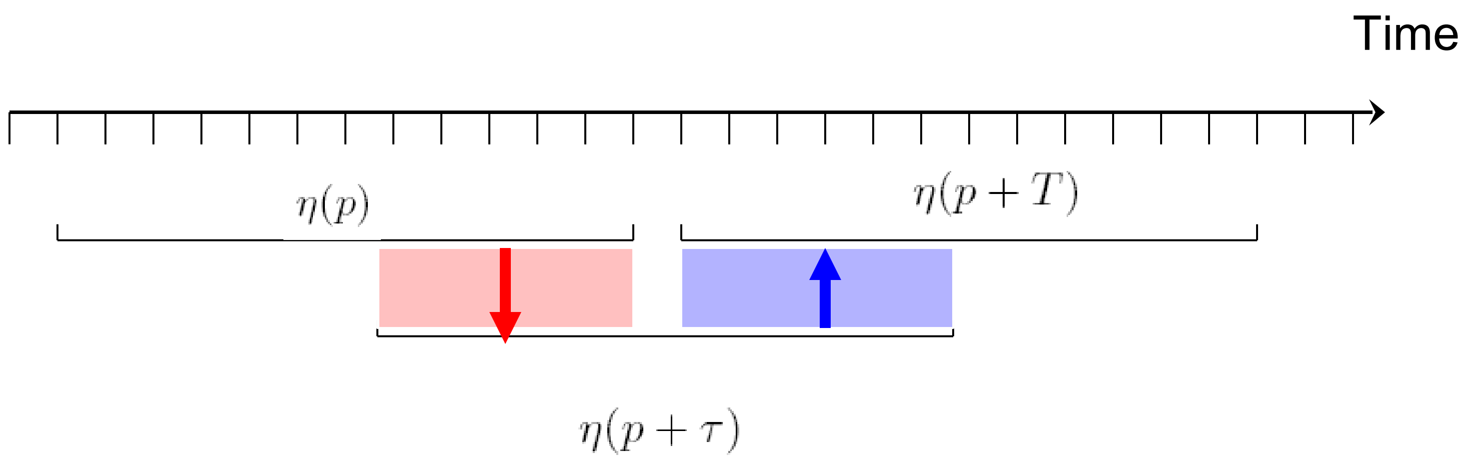
$$\mathcal{W}_{ij}^{(n)} = \mathcal{W}_{ij}^{(n-1)} + \mathcal{R}_{ij}(s_\lambda),$$

$$\mathcal{W}_{ij}^{(0)} = \delta_{ij} - \sum_{n=1}^{N} \mathcal{R}_{ij}(s_n),$$

$$\eta_j^{(0)}(p) = 0$$

Sequential Model : Long-Term Prediction

- Model can also be used for long-term prediction.
- Information between non overlapping episodes is passed through *"bridging"*.



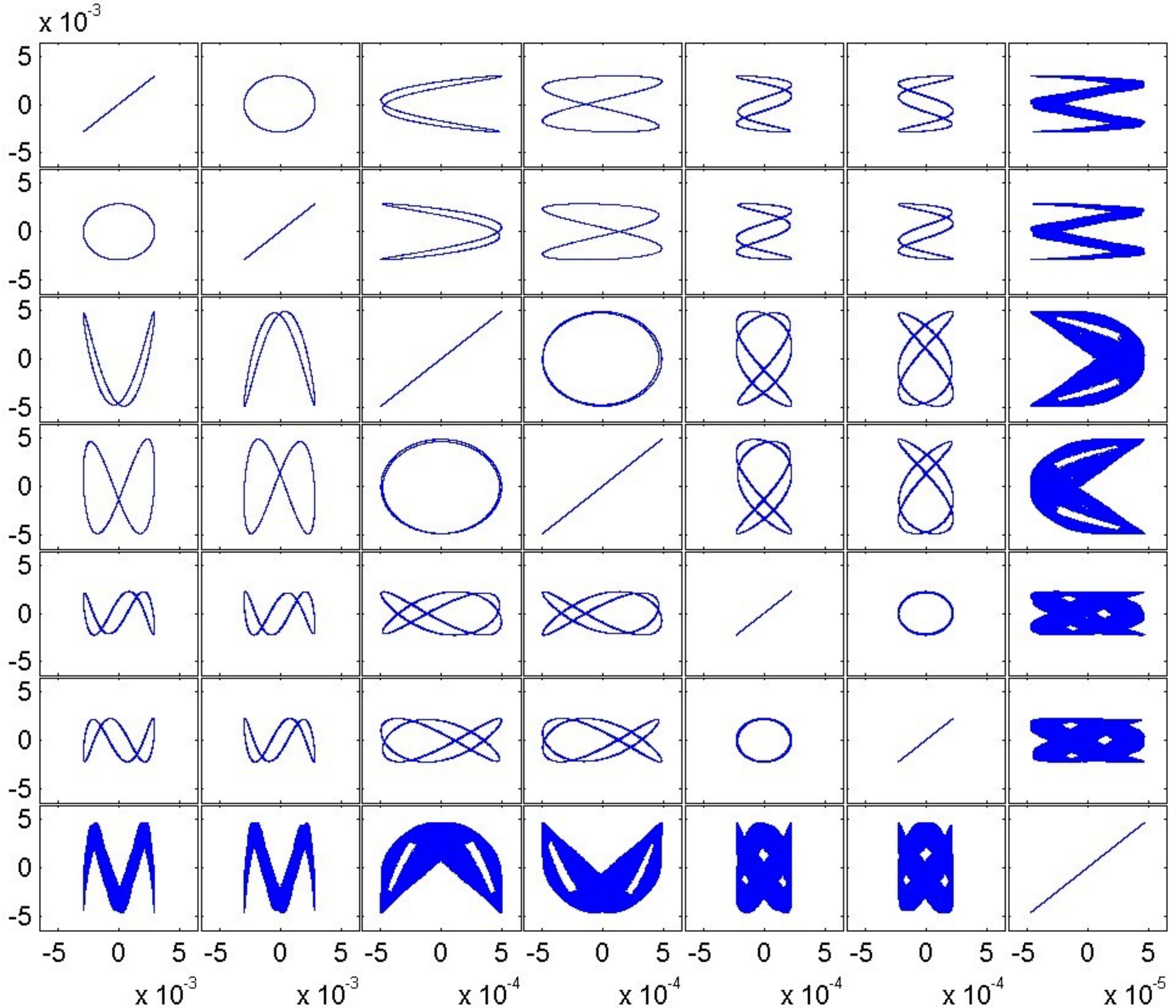
Examples

- Flow around 2D cylinder.
  - Re = 100, shedding frequency = 10 Hz
  - Snapshots available every 0.0001 seconds
  - Snapshots/Episode = 100
- 9D chaotic Lorenz model
  - Snapshots available every 0.5 seconds
  - Snapshots/Episode = 200

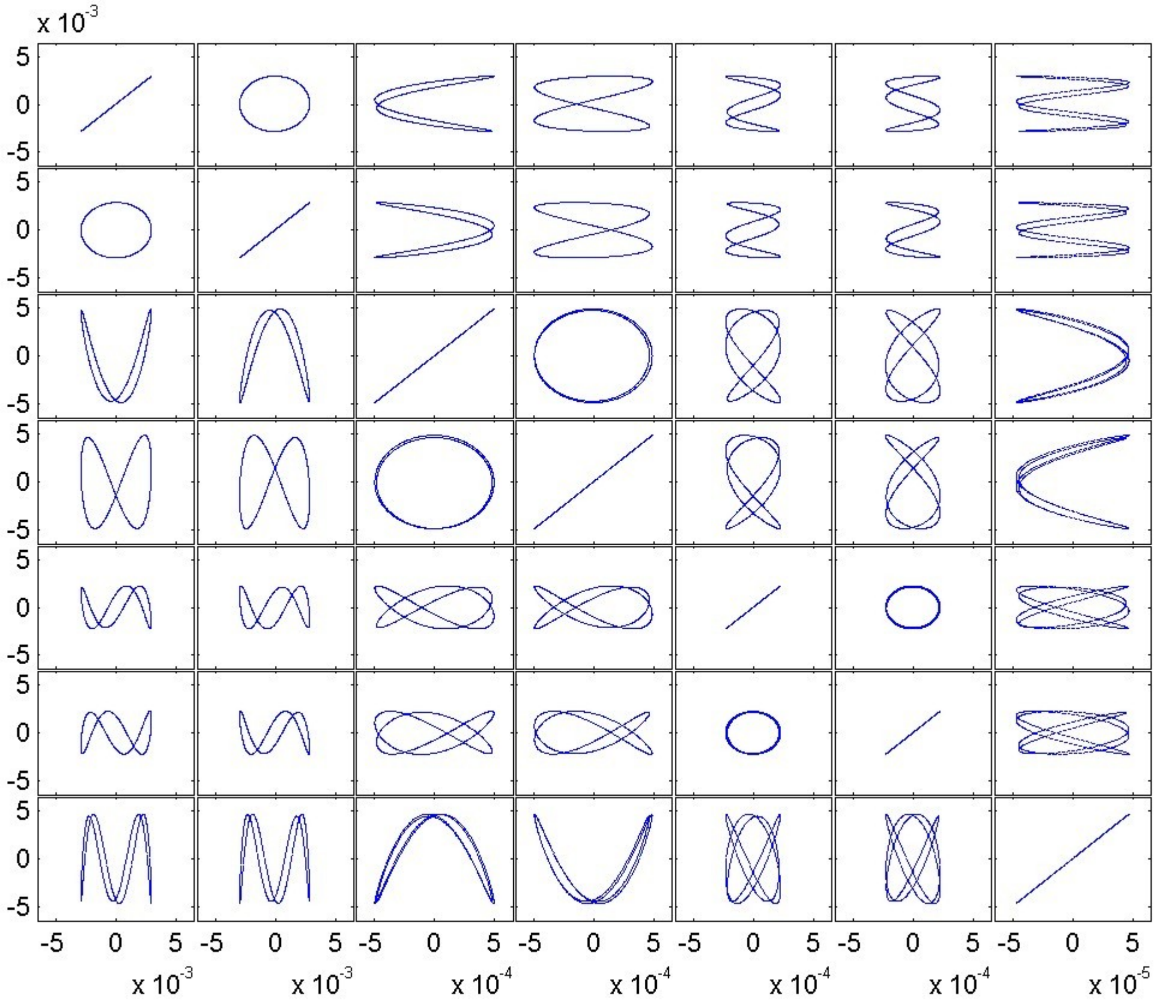
Example – 2D Cylinder

- Example is used to test accuracy of long-term prediction
- POD coefficients are predicted for 5000 shedding cycles
- Initial condition at some random time is provided
- Results compared with solution obtained from quadratic system of ODEs (Galerkin model)

Example – 2D Cylinder (Galerkin Mo



Example – 2D Cylinder (Ep-POD Mo



Example 2 – 9D Lorenz Model

$$\dot{C}_1 = -\sigma b_1 C_1 - C_2 C_4 + b_4 {C_4}^2 + b_3 C_3 C_5 - \sigma b_2 C_7$$
$$\dot{C}_2 = -\sigma C_2 + C_1 C_4 - C_2 C_5 + C_4 C_5 - \sigma C_9/2$$
$$\dot{C}_3 = -\sigma b_1 C_3 + C_2 C_4 - b_4 {C_2}^2 - b_3 C_1 C_5 + \sigma b_2 C_8$$
$$\dot{C}_4 = -\sigma C_4 - C_2 C_3 - C_2 C_5 + C_4 C_5 + \sigma C_9/2$$
$$\dot{C}_5 = -\sigma b_5 C_5 + {C_2}^2/2 - {C_4}^2/2$$
$$\dot{C}_6 = -b_6 C_6 + C_2 C_9 - C_4 C_9$$
$$\dot{C}_7 = -b_1 C_7 - r C_1 + 2 C_5 C_8 - C_4 C_9$$
$$\dot{C}_8 = -b_1 C_8 + r C_3 - 2 C_5 C_7 + C_2 C_9$$
$$\dot{C}_9 = -C_9 - r C_2 + r C_4 - 2 C_2 C_6 + 2 C_4 C_6 + C_4 C_7 - C_2 C_8.$$

$$b_1 := 4\frac{1+a^2}{1+2a^2} \qquad b_2 := \frac{1+2a^2}{2\left(1+a^2\right)} \qquad b_3 := 2\frac{1-a^2}{1+a^2}$$
$$b_4 := \frac{a^2}{1+a^2} \qquad b_5 := \frac{8a^2}{1+2a^2} \qquad b_6 := \frac{4}{1+2a^2}.$$

$$a = \tfrac{1}{2} \qquad \sigma = 0.5 \qquad r = 14.22$$

Example 2 – 9D Lorenz Model

- Episodic length = 200 time steps
- Example used to test sequential model and its robustness to outliers
- Two tests are performed:
  - Ep-POD model is provided with coefficients every 40 time steps
  - Ep-POD model is provided with noisy coefficients every 20 time steps. Noise is white noise with standard deviation of 0.2
- Evolution of the coefficients is tracked for 1200 time steps

Example 2 – 9D Lorenz Model (no noise)

Example 2 – 9D Lorenz (with noise)

REMARKS

- Ep-POD sequential model is found to be robust and is dynamically consistent
- Linear formulation makes implementation fast
- Models work especially well for strongly periodic cases
- Ep-POD model behaves similar to a linear Kalman filter

REMARKS

- Currently, episodic length is set equal to the dominant frequency in the flow
- Effect of episodic length needs to be studied
- Selection of episodic length needs to addressed more rigorously
- Model has been tested for very high dimensional models

Predicting Complex Flows
Part II:
Radial Basis Function Approach to Modeling Dynamical Systems

Introduction

- Consider a time series given by

$$\zeta_k(t_i),\ \ i = 1, 2, ...M,\ \ k = 1, 2, ..., N$$

- The time series follows from a dynamical system given by

$$\frac{d\zeta_k}{dt} = \sum_{i=1}^{N}\sum_{j=1}^{N} A_{kij}\zeta_i\zeta_j + \sum_{l=1}^{N} B_{kl}\zeta_l.$$

Introduction

- We are interested in the modeling the evolution of $\zeta_k(t)$
- Given:
  - Sample time series
  - Time derivatives or pair-wise time series
- The model is derived from the concept of surface approximation using radial basis functions

RBF-Based Model

- RBF model takes the form of

$$g_s(\overline{\zeta}^n) = \sum_{k=1}^{N} \mathcal{R}_{sk}\zeta_k + \sum_{j=1}^{M} \lambda_{sj}\ \Phi(||\boldsymbol{c}^j - \overline{\zeta}^n||_2)$$

- where

$$\Phi_j(\boldsymbol{x}) = e^{(-\epsilon^2\ ||\boldsymbol{x}-\boldsymbol{c}_j||_2^2)},\ \text{Gaussian Function},$$

$$\Phi_j(\boldsymbol{x}) = \sqrt{1+\epsilon^2\ ||\boldsymbol{x}-\boldsymbol{c}_j||_2^2},\ \text{Multi-quadric function},$$

$$\Phi_j(\boldsymbol{x}) = \frac{1}{\sqrt{1+\epsilon^2\ ||\boldsymbol{x}-\boldsymbol{c}_j||_2^2}},\ \text{Inverse multi-quadric function.}$$

RBF-Based Model

- The coefficients in the RBF model are solved via a system of linear equations

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \lambda \\ \mathcal{R} \end{bmatrix} = \begin{bmatrix} g \\ h \end{bmatrix}$$

RBF-Based Model

$$A = A_{ij} = \Phi(||\overline{\zeta}(t_i) - \overline{\zeta}(t_j)||_2),\ i = 1,2...M,\ j = 1,2,..M,$$

$$B = B_{im} = \zeta_m(t_i),\ i = 1,2,...,M,\ m = 1,2,...N,$$

$$g = g_s(\overline{\zeta}(t_i)),\ i = 1,2,....,M.$$

$$C_{kl} = \sum_p Q_{lp} g_k(t_p),\ l = 1,2,...,M,\ k = 1,2,.....N$$

$$D_{kr} = \sum_p \zeta_r(t_p) g_k(t_p),\ r = 1,2,....N,\ k = 1,2,....N,$$

$$h_{ks} = \sum_p g_k(t_p) g_s(t_p),\ k = 1,2,...,M,\ s = 1,2,.....M$$

$$Q_{lp} = \left[\sum_{k=1}^{N}\left[\zeta_k(t_p)\ \left(\frac{\partial\Phi_l}{\partial\zeta_k}\right)_{\overline{\zeta}^n=0} + \frac{1}{2}(\zeta_k(t_p))^2\ \left(\frac{\partial^2\Phi_l}{\partial\zeta_k^2}\right)_{\overline{\zeta}^n=0}\right] + \sum_{i=1}^{N}\sum_{j=i}^{N}(\zeta_i(t_p)\ \zeta_j(t_p))\ \left(\frac{\partial^2\Phi_l}{\partial\zeta_i\partial\zeta_j}\right)_{\overline{\zeta}^n=0}\right]$$

$$\Phi_l = \Phi(||\overline{\zeta}(t_l)||_2).$$

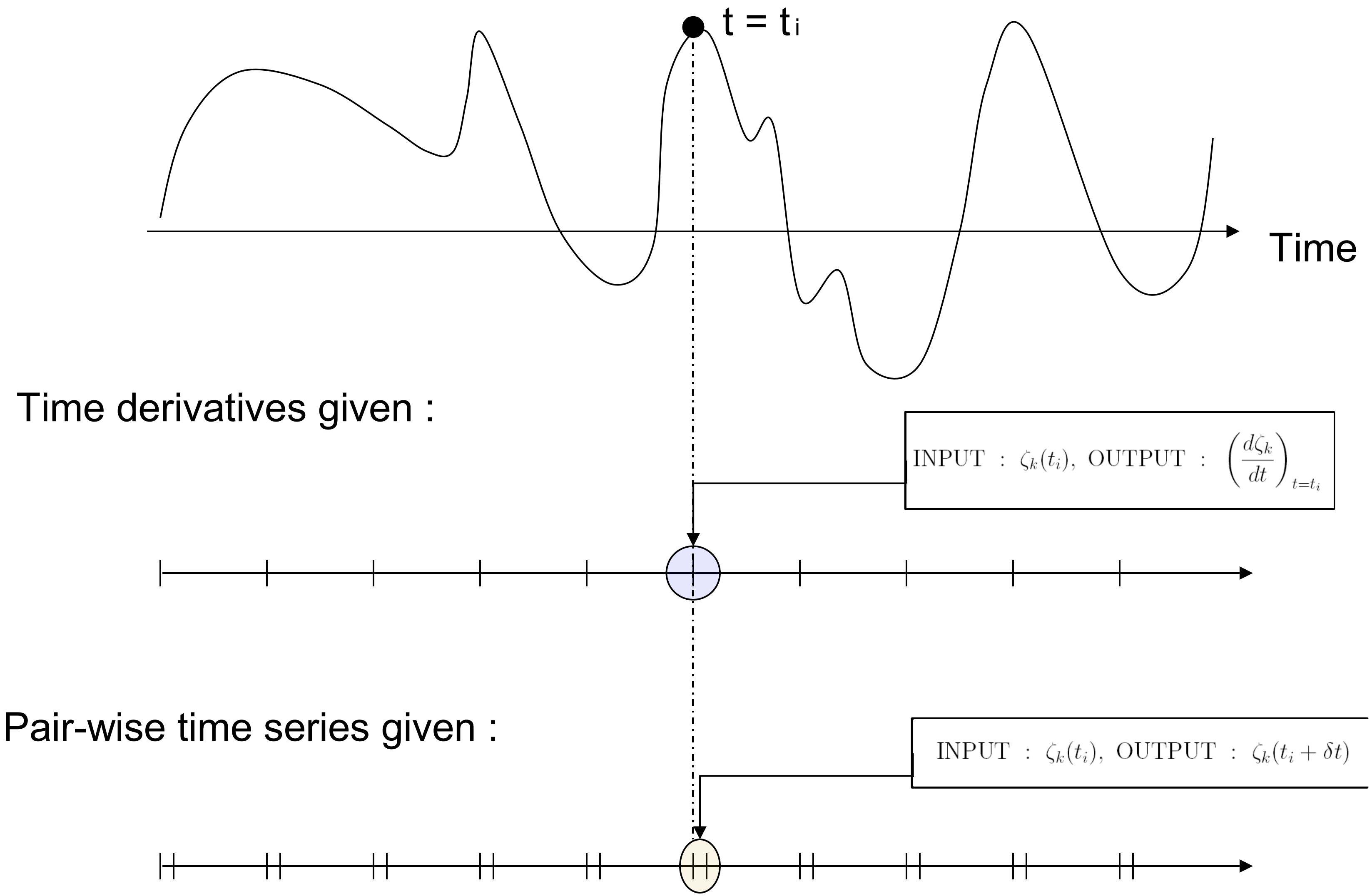
RBF-Based Model

- If continuous derivatives are given, then

$$g_s(\overline{\zeta}(t_i)) = \left(\frac{d\zeta_s}{dt}\right)_{t=t_i}$$

- If pair-wise time series is given, then

$$g_s(\overline{\zeta}(t_i)) = \zeta_k(t_i + \delta t)$$



t = tᵢ
Time
Time derivatives given :
INPUT : $\zeta_k(t_i)$, OUTPUT : $\left(\frac{d\zeta_k}{dt}\right)_{t=t_i}$
Pair-wise time series given :
INPUT : $\zeta_k(t_i)$, OUTPUT : $\zeta_k(t_i + \delta t)$

Examples

- Three examples are considered
  - 3D Lorenz model
  - 9D Lorenz model
  - Kuramoto-Sivashinsky model
- RBF models are generated for the continuous and discrete cases using sample time series
- Time evolution of the model variables is compared

Example – 3D Lorenz Model

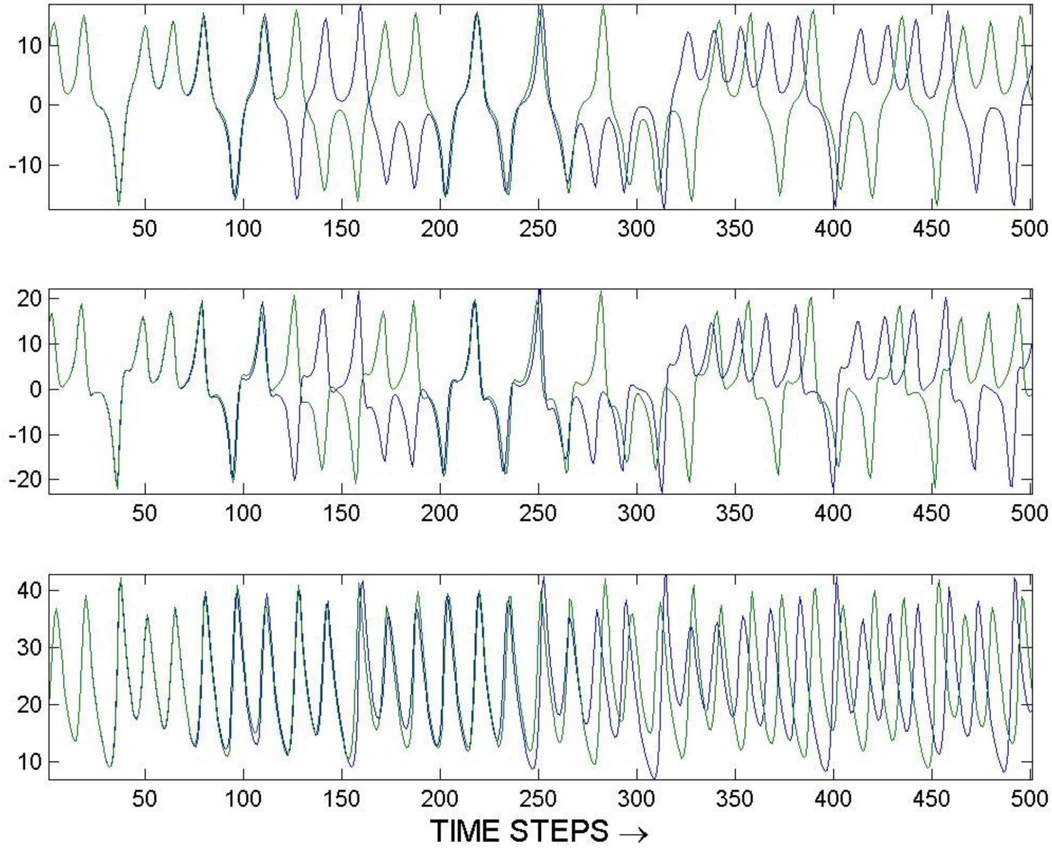
- 3D Lorenz model is given by

$$\frac{dx_1}{dt} = \sigma(x_2 - x_1),$$
$$\frac{dx_2}{dt} = -x_2 - x_1 x_3 + \alpha x_1,$$
$$\frac{dx_3}{dt} = x_1 x_2 - \beta x_3,$$

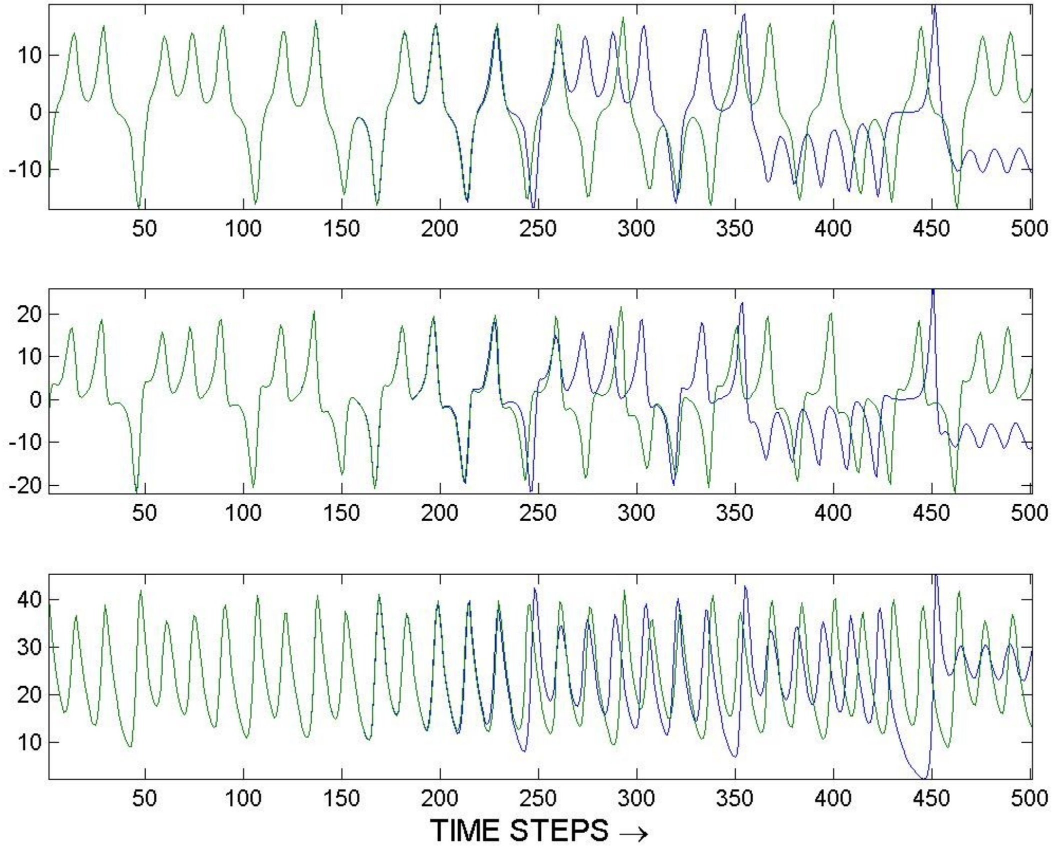
$$\sigma = 10, \ \alpha = 28, \ \beta = 8/3.$$

- 200 time steps of sample time series is used to generate RBF model

Example – 3D Lorenz Model (time derivatives given)



Example – 3D Lorenz Model (Pair-wise time series given)



Example – 9D Lorenz Model

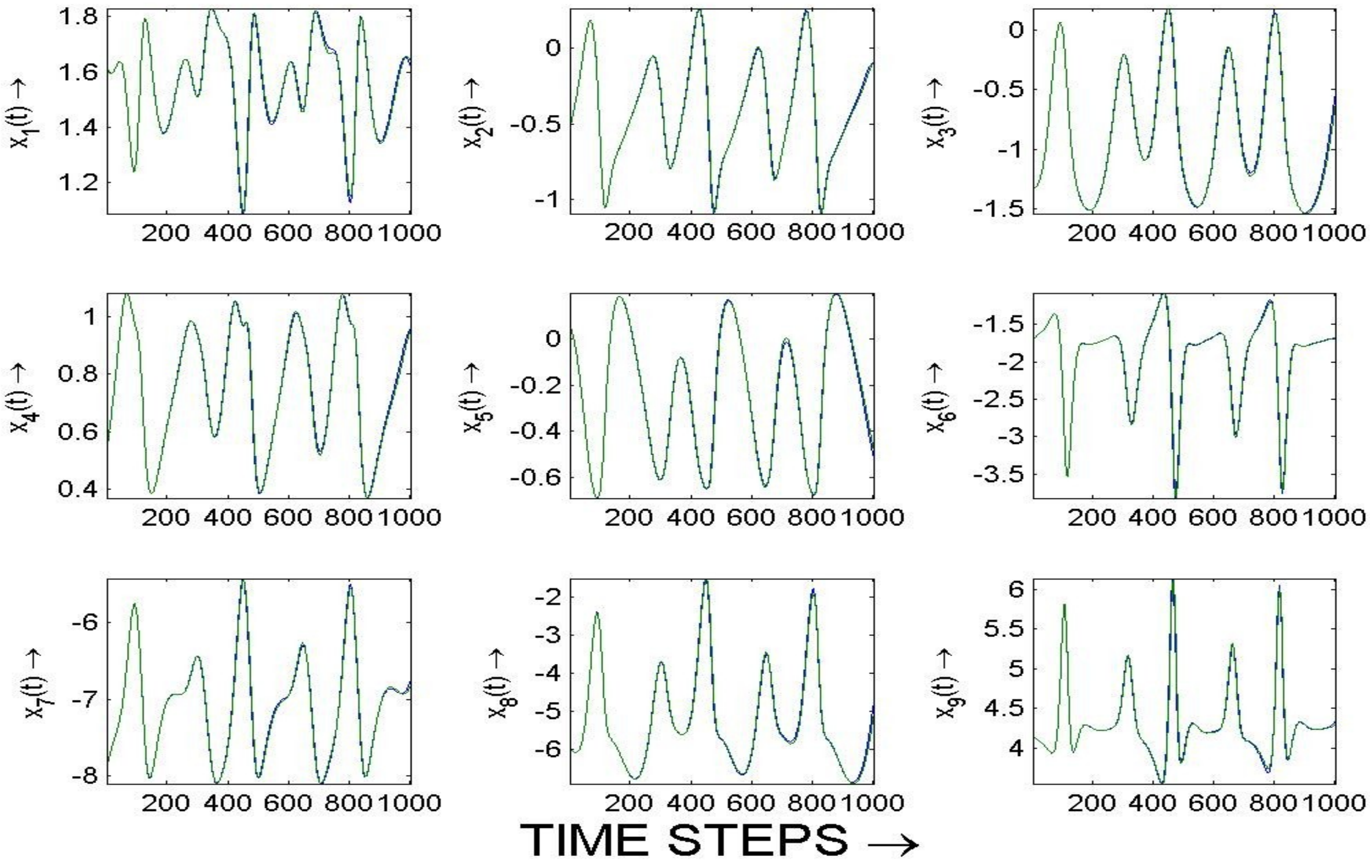
- 500 time steps of sample time series used to generate RBF model.
- 9D Lorenz model is given by

$$\dot{C}_1 = -\sigma b_1 C_1 - C_2 C_4 + b_4 {C_4}^2 + b_3 C_3 C_5 - \sigma b_2 C_7$$
$$\dot{C}_2 = -\sigma C_2 + C_1 C_4 - C_2 C_5 + C_4 C_5 - \sigma C_9/2$$
$$\dot{C}_3 = -\sigma b_1 C_3 + C_2 C_4 - b_4 {C_2}^2 - b_3 C_1 C_5 + \sigma b_2 C_8$$
$$\dot{C}_4 = -\sigma C_4 - C_2 C_3 - C_2 C_5 + C_4 C_5 + \sigma C_9/2$$
$$\dot{C}_5 = -\sigma b_5 C_5 + {C_2}^2/2 - {C_4}^2/2$$
$$\dot{C}_6 = -b_6 C_6 + C_2 C_9 - C_4 C_9$$
$$\dot{C}_7 = -b_1 C_7 - r C_1 + 2 C_5 C_8 - C_4 C_9$$
$$\dot{C}_8 = -b_1 C_8 + r C_3 - 2 C_5 C_7 + C_2 C_9$$
$$\dot{C}_9 = -C_9 - r C_2 + r C_4 - 2 C_2 C_6 + 2 C_4 C_6 + C_4 C_7 - C_2 C_8.$$

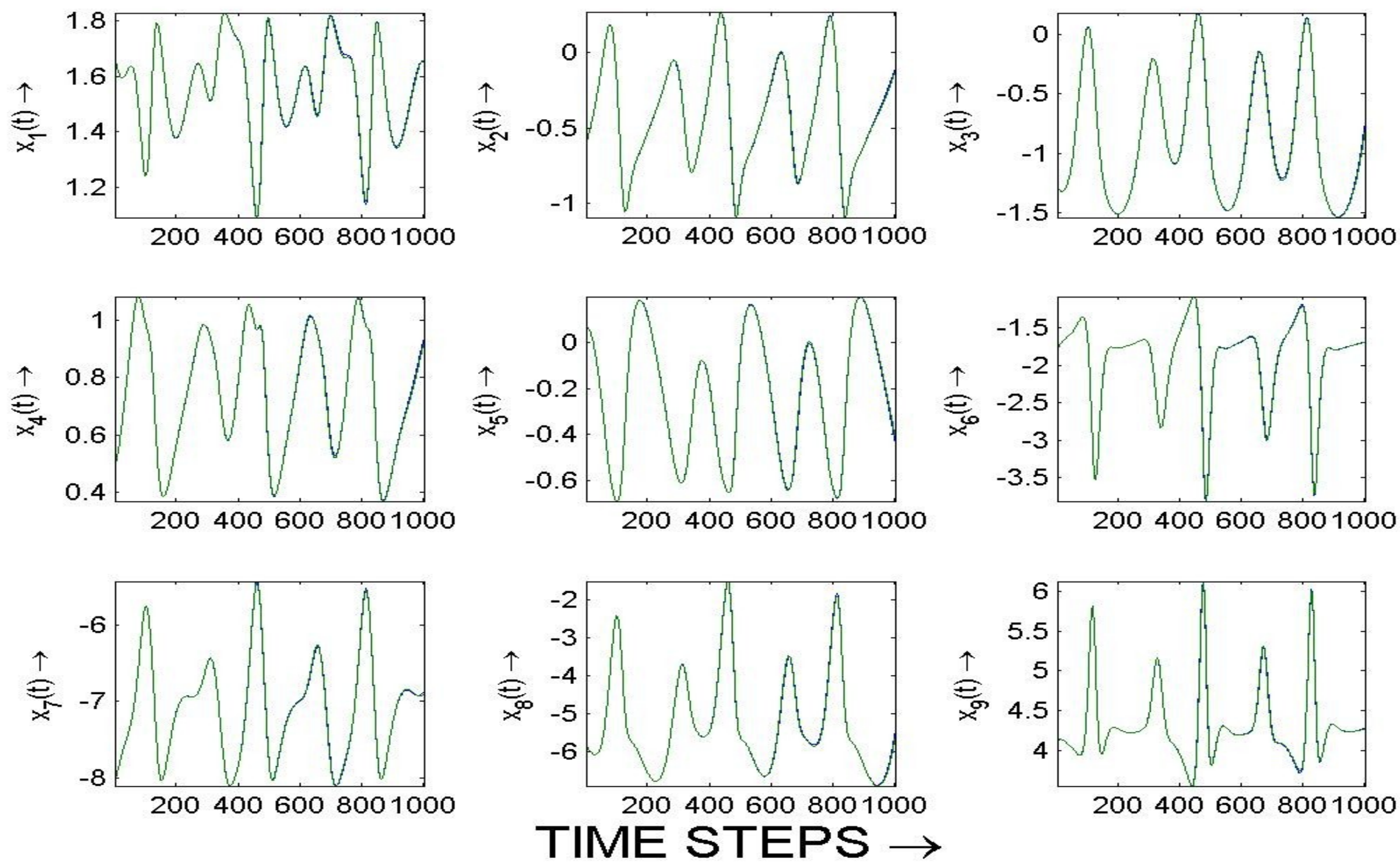
$$b_1 := 4\frac{1+a^2}{1+2a^2} \qquad b_2 := \frac{1+2a^2}{2\left(1+a^2\right)} \qquad b_3 := 2\frac{1-a^2}{1+a^2}$$
$$b_4 := \frac{a^2}{1+a^2} \qquad b_5 := \frac{8a^2}{1+2a^2} \qquad b_6 := \frac{4}{1+2a^2}.$$

$$a = \tfrac{1}{2} \qquad \sigma = 0.5 \qquad r = 14.22$$

Example – 9D Lorenz Model (time derivatives given)



Example – 9D Lorenz Model (pair-wise time series given)



Example – KS Equation

- Governing equation

$$\frac{\partial u}{\partial t} = -u\,\frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^4 u}{\partial x^4}$$

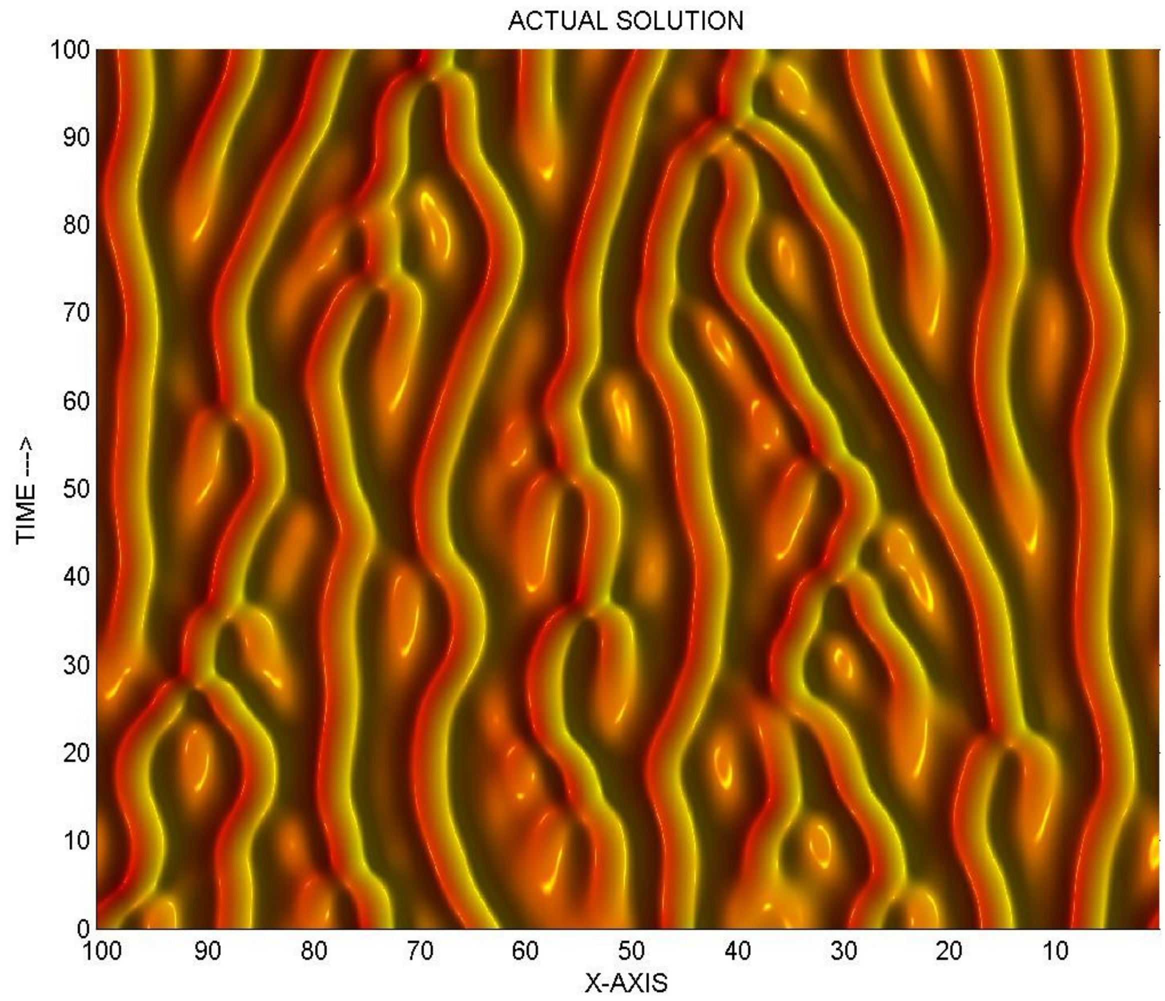
- Low-dimensional form identical to Navier-Stokes equation
- Periodic boundary conditions
- Space: Fourier decomposition
- Time: Exponential time differencing with RK-4 scheme
- Initial condition

$$u(x, t = 0) = \cos(\frac{x}{8})(1 + \sin(\frac{x}{8}))$$

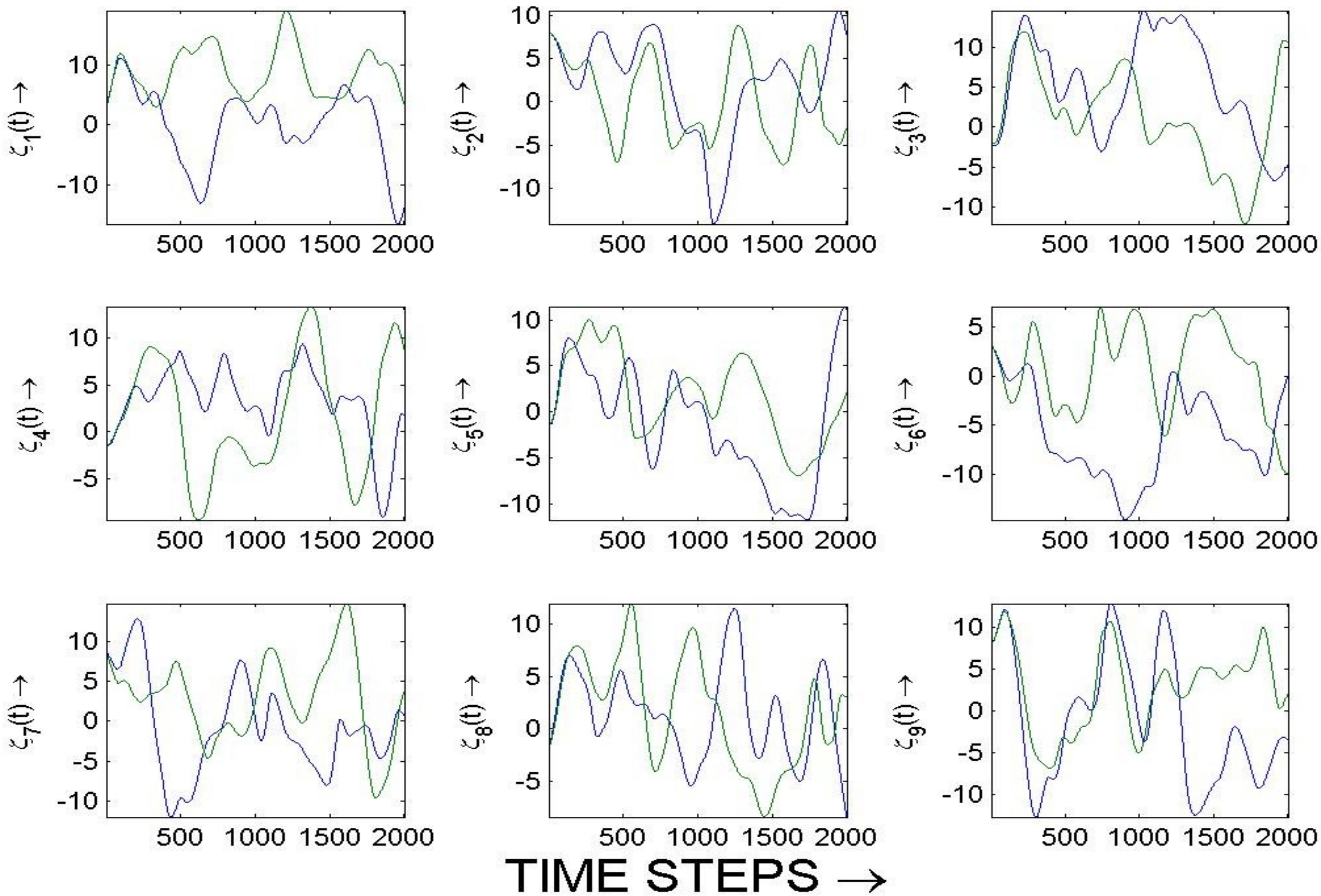
Example – KS Equation

- POD analysis is done on the solution
- 75 POD modes used to construct dynamical system
- Each differential equation has 2925 terms
- 2000 time steps of sample time series at interval of 1 is used
- Parameter estimation using least-squares leads to highly under-determined system of equations

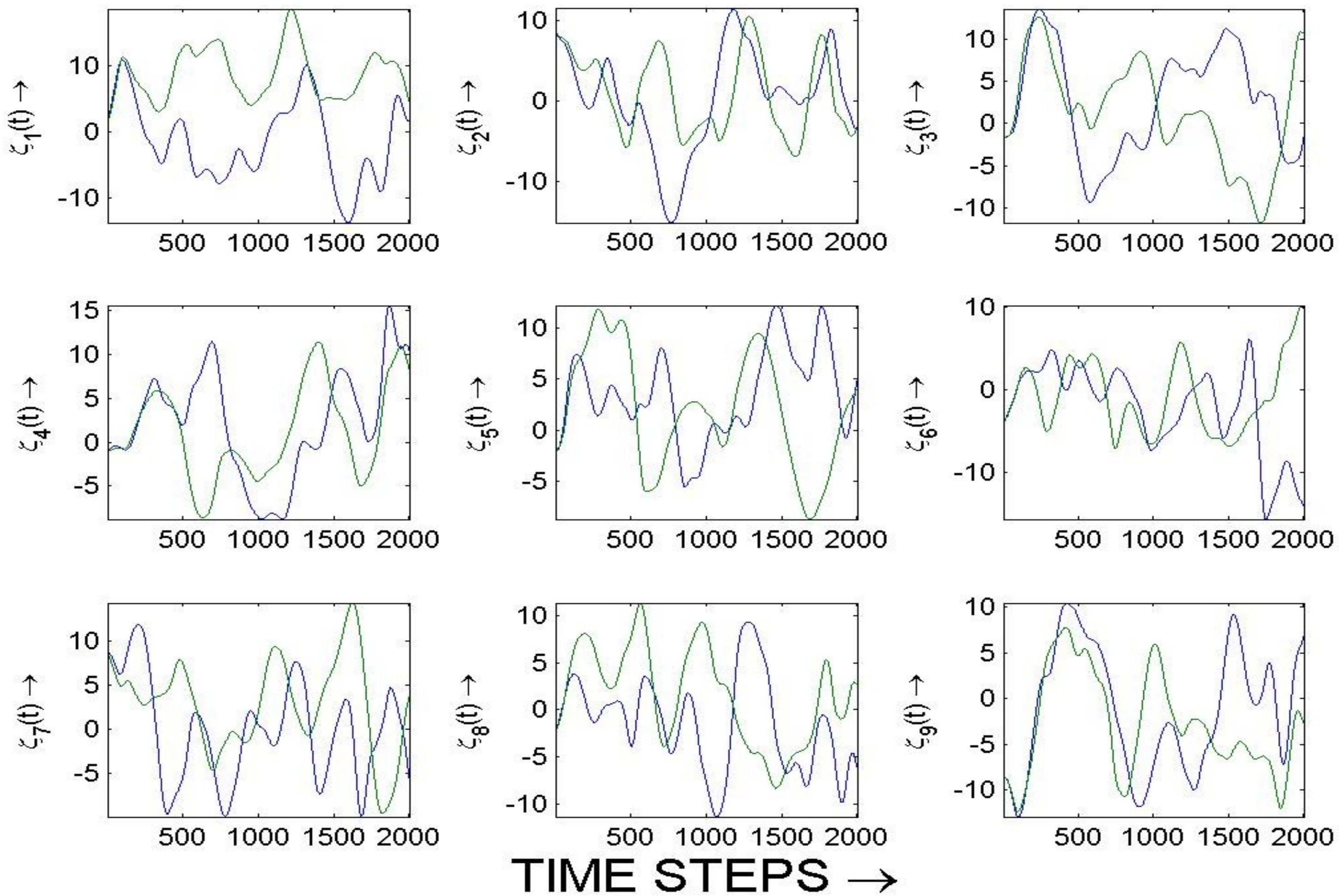
KS Equation Solution



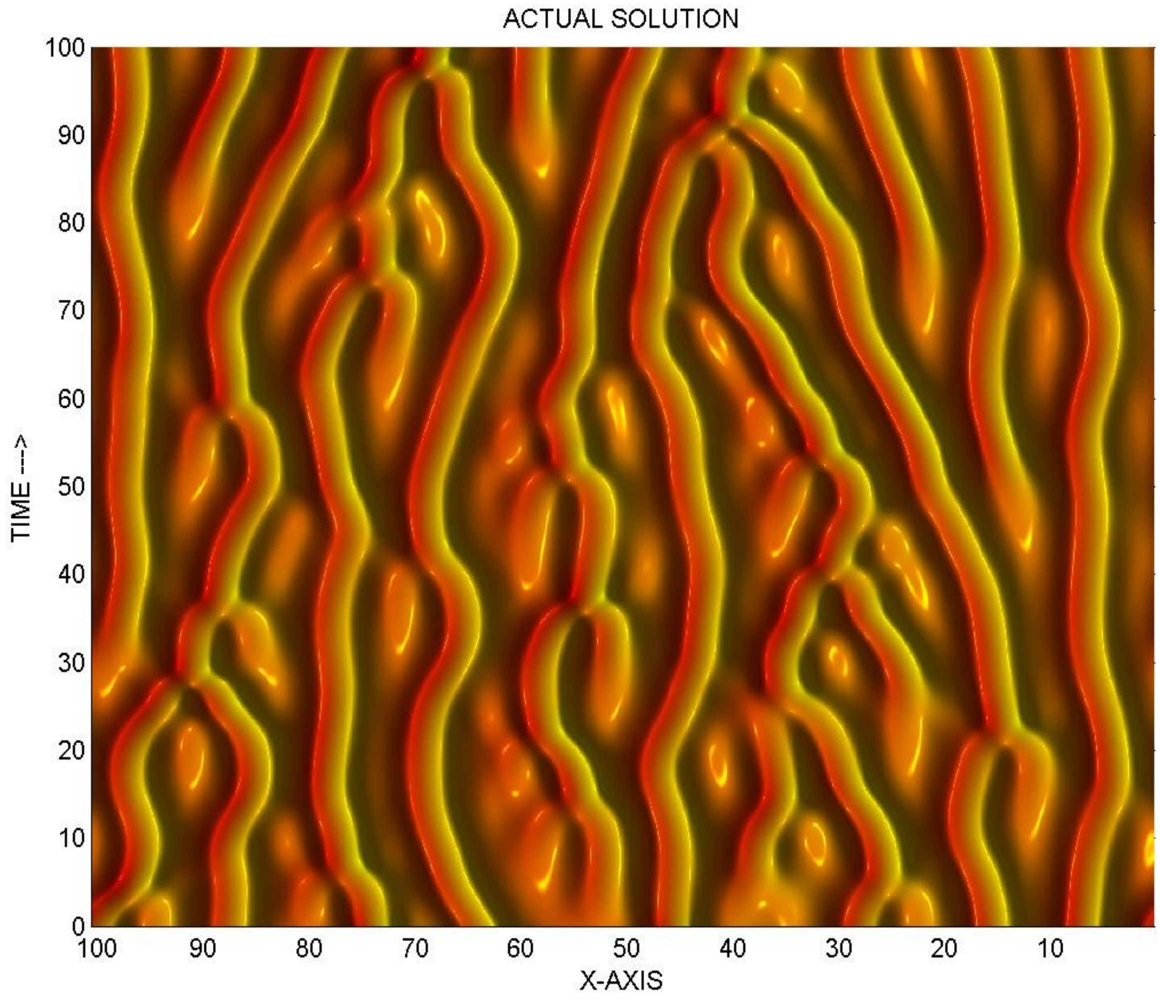
KS Equation (time derivatives given)



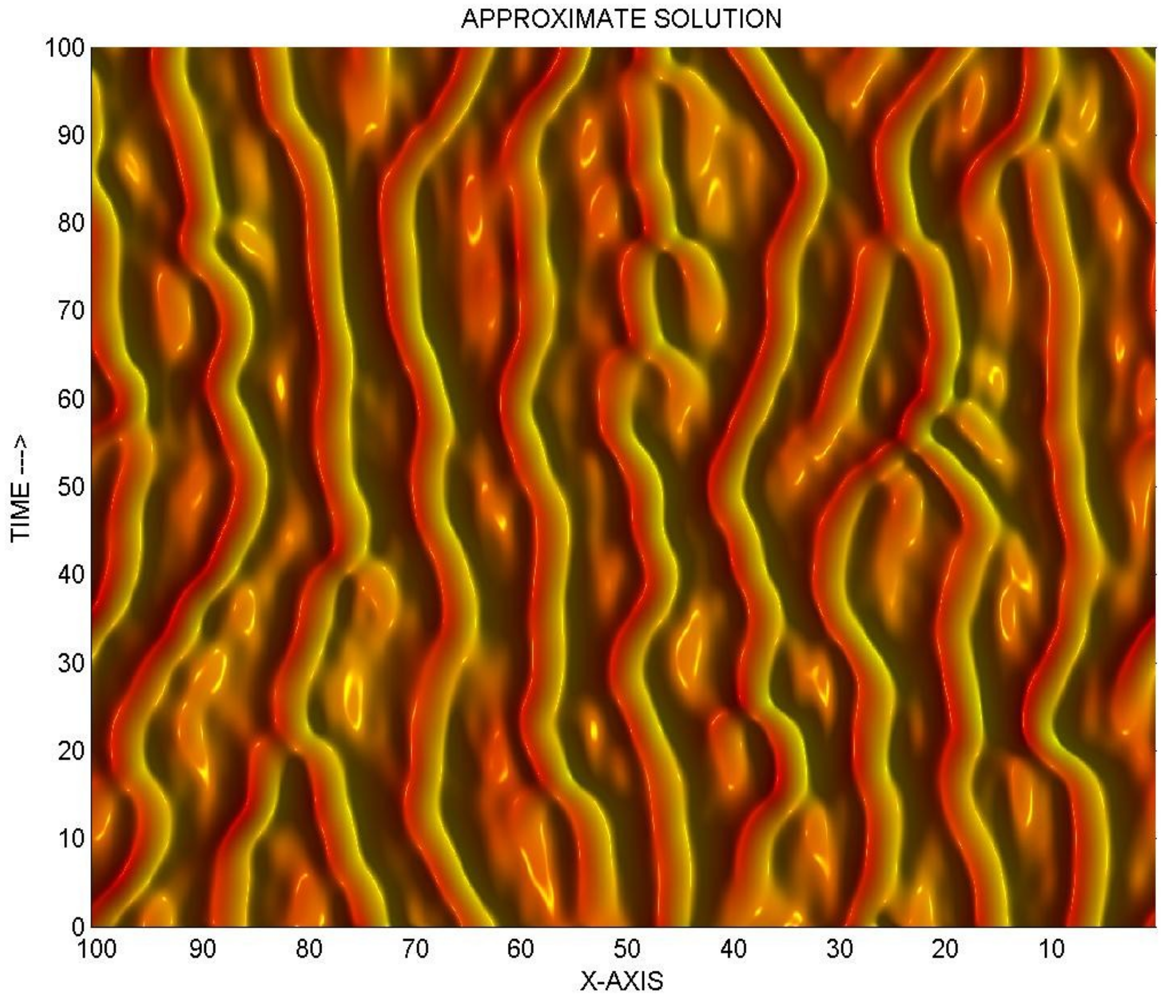
KS Equation (pair-wise time series)



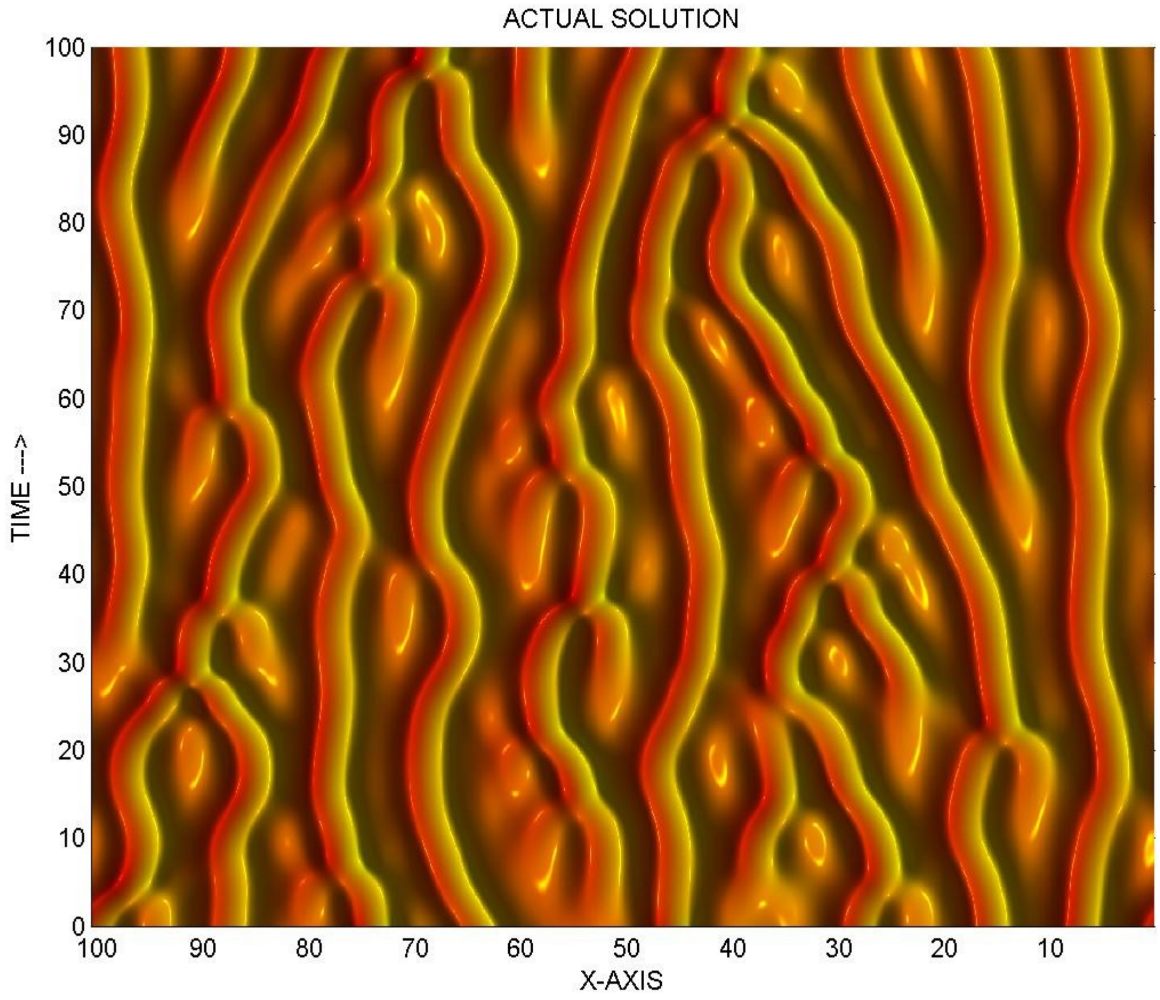
KS Equation Solution



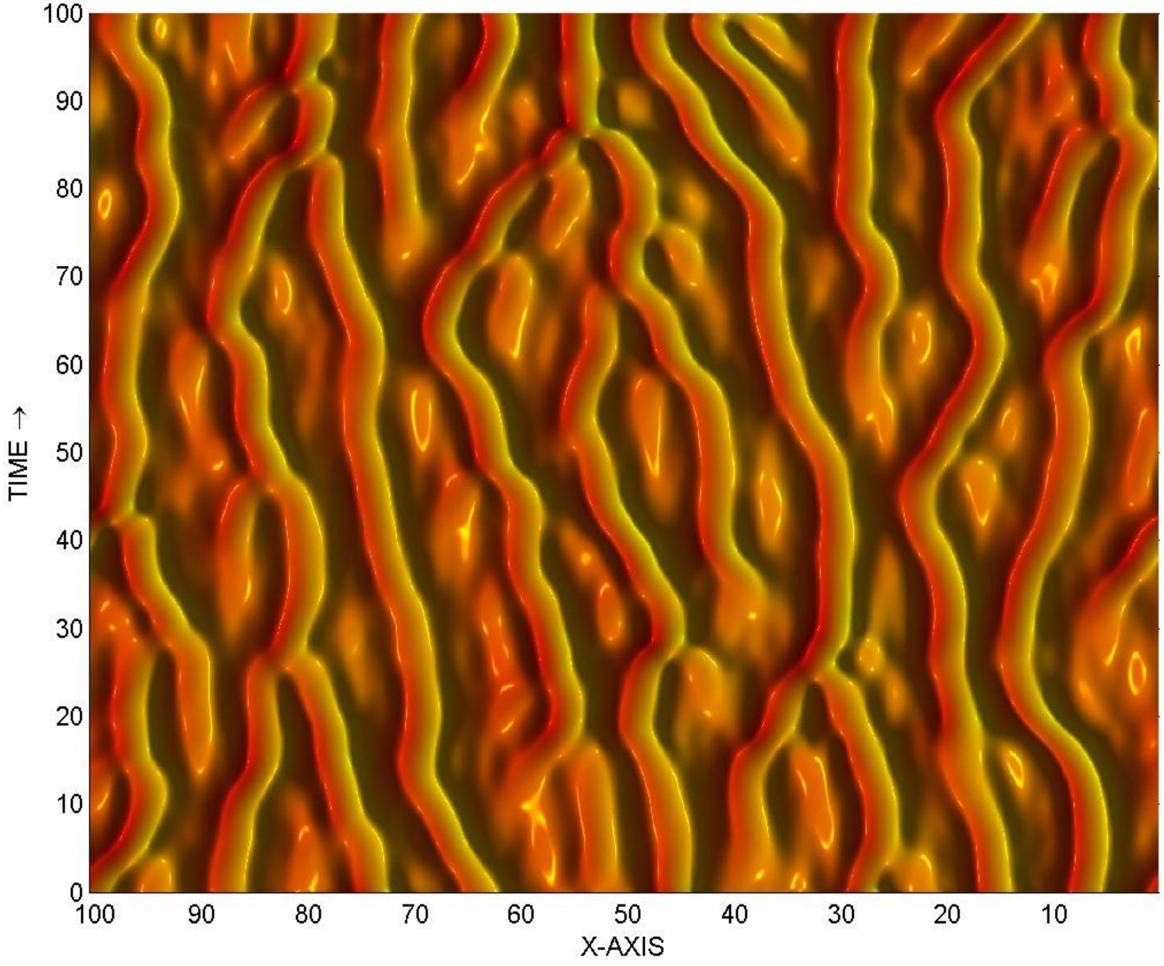
KS Equation (time derivatives given)



KS Equation Solution



KS Equation (pair-wise time series)



QUESTIONS ….?