Chapter 6

Conclusion and Future Scope

Studies in chaos theory have enhanced the scope of studying irregular time series data obtained from experiments. The studies in this area provide deep connections between empirical observations and theory as typically shown in Chapter 2 where using experimental time series observations of stress measurements in an aqueous polymer solution (N-isopropyl acrylamide) and a biopolymer (Carrageenan) showed irregularity for identifiable steady shear regions. A way to efficiently preprocess the data by noise reduction for enhancing systemic features using wavelet transform was also developed. The noise reduction was carried out efficiently by differentiating the stress measurement data and subjecting this differentiated data to wavelet transform. The process of carrying out the wavelet transform shifts the power due to noise to the lower wavelet scales and these could be automatically identified from the power spectrum of the wavelet coefficients at the different scales. Noise free and feature enhanced time series data could be obtained by setting the wavelet coefficients in these lower wavelet scales to zero before inverse wavelet transform and integration. The noise free data was subsequently used for characterization of the dynamical properties of the systems under consideration. Interesting theoretical conclusions about the nature of the experimental systems being studied have thus been presented. The analysis of the denoised rheological data using phase-space reconstruction techniques, in fact, revealed
the presence of low-dimensional attractors as can be obtained from studies with two model reacting systems, namely, endo-exothermic and autocatalytic reactions taking place in a CSTR and exhibiting chaotic dynamics. The presence of chaotic dynamics was established by studying invariant properties of the observed dynamics with respect to the mutual information, correlation dimension, Lyapunov exponents and entropy. Lyapunov dimension for these low dimensional systems turned out to be less than 3 which suggested the presence of a strongly contracting flow and that valuable information about the chaotic dynamics could be gained by additionally carrying out a topological analysis of the observed attractors. The topological analysis required the identification of periodic orbits from the first return map on the Poincarè section and the method to achieve this has been described. A topological study of the extracted periodic orbits showed global characterization and classification of dynamics was indeed possible using topological invariants, namely, linking numbers and relative rotation rates. The topological entropy was also calculated and it converged to a value comparable to entropy estimated from Lyapunov spectrum showing the robustness in the methodologies used for topological characterization. Analysis of these invariants also yielded the template and the Markov transition matrix that contained in them the basic nature of the flow. It was observed that the template could be deduced by topological characterization of only the period-1, 2 and 3 orbits. Interestingly, results of analysis showed that both the experimental and the model system considered followed the Horseshoe mechanism in terms of stretching and folding associated with chaotic dynamics. The results show how properties of systems in interdisciplinary areas are related due to existence of universal properties and that systems of interest in many physical and chemical systems exhibiting chaotic dynamics may be classified and studied on common grounds.

Reaction-diffusion-convection systems are particularly interesting and may be modeled with optimum dimensionality by Galerkin projection of the original high-
dimensional model as shown in Section 5.1. It is interesting to note that reduced models of spatiotemporal systems exhibit features like synchronization properties of low-dimensional chaotic systems as seen in Section 5.3. Characterization and quantification of spatiotemporal chaos can be further pursued by analyzing these finite-dimensional systems. However, topological analysis discussed in Section 2.3.2 holds good for dynamical systems for the Lyapunov dimension $d_L < 3$. Locating periodic orbits and their surrogates for high-dimensional system is also difficult because the unstable periodic orbits fall apart when embedding dimension $m > 3$. This suggests topological invariants need new formalisms like consideration of subsystems for high-dimensionality. Extending the topological analysis to high-dimensional system will throw some light in understanding transition routes to spatiotemporal chaos, pattern formation, intermittency, turbulence, etc. It is hoped that with the methodologies presented here, these topics may be addressed with success in the near future.

The invariant measures analyzed above depend upon the parameter values of the system. A knowledge of these parameter values is essential for studying system properties and the behavior of the models with respect to stability, bifurcation, control, etc. Thus, it is important to estimate the values of unknown parameters of the system by auto tuning an appropriate nonlinear model to fit the observed chaotic data. Chapter 3 considered the simple situation of a well-mixed system whose dynamics is described by a set of coupled nonlinear ordinary differential equations. Developing boundary value multiple shooting approach to parameter estimation, was chosen so that its logical extension for applications in high-dimensional systems could be carried out. It may be emphasized that for chaotic dynamics, estimating parameters and system states is not a trivial task even for simple model descriptions. The results presented focus on this practically important aspect of modeling and bring out the advantages gained by applying the boundary value multiple shooting approach to stringent nonlinear situations when the system exhibits low-dimensional chaotic
dynamics. The aim here, therefore, was to simultaneously estimate all values of the unknown parameters and non-monitored system states from available transient data. Further exemplification of the analysis was carried out by adapting the method to tune empirical mathematical models using scalar time series with noisy data. The results of estimating all intrinsic kinetic parameters and operational system parameters even with small data sets show the robustness and usefulness of the methodology.

Chapters 4 and 5 study the class of complex systems, that show not only temporal variability but also spatial. The variability in these spatially extended systems are brought about by reaction-diffusion-convection mechanisms operating in the process. Unlike temporal systems that could be modeled as ordinary differential equations as in Chapters 2 and 3, reaction-diffusion-convection systems need to be modeled by partial differential equations due to the introduction of the spatial domain. Spatiotemporal systems can be studied using CML models which show the necessary complex spatiotemporal features like chaos, traveling wave, etc. They are popularly used in studies because the ease in computation affords methodologies and analysis of complex system dynamics to be well developed before applying them to continuous time domain systems which are less tractable. All the same, studies with CML's is not easy due to the high-dimensionality introduced by the spatial domain and the nonlinear mechanisms operating. In this scenario, it was found advantageous to identify the coherent spatial structures present in the space-time data so that a separable form of the CML model amenable to dimensionality reduction (i.e. model reduction) could be obtained. The identification of coherent structures could be carried out by calculating empirical eigenfunctions from the correlation matrix obtained from the space-time data and using Karhunen-Loève (KL) decomposition. The results obtained for the representative systems, namely, CML, an autocatalytic and an activator-inhibitor systems for different types of complex dynamics showed when and to what extent model reduction is possible. These results are discussed in detail in

121
Chapter 4. Importantly, we also studied situations when incomplete spatiotemporal information is only available due to partial monitoring. Here, the aim was to reconstruct masked portions of the data while carrying out the projection. The method when applied to situations where snapshots in time are marred with noise successfully yielded unbiased estimates of the missing information using the evaluated empirical eigenfunctions.

Importantly, it was possible to design ways of applying the low-dimensional methodologies discussed in Chapters 2 and 3 for the high-dimensional spatiotemporal systems that have been considered. This was made possible by model projection techniques using Galerkin's method on the separable model obtained by KL decomposition. The profitable use of this approach is seen when the methodology of multiple shooting studied in Chapter 3 can be reformulated to estimate all parameters of the high dimensional system using KL reduced model descriptions with Galerkin projection. In Chapter 5 we have developed the Karhunen-Loève and Galerkin multiple shooting (KLGMS) approach and have exemplified it for both coupled map lattice (CML) systems and the two reacting systems. The resulting advantages in estimating parameters from small amounts of data from subsystems (i.e. local regions/channels), availability of only scalar and noisy time series data, effects of space time parameter variations and in the presence of multiple time scales was significantly demonstrated. Apart from empirical eigenfunctions, the use of wavelet basis functions as a complementary alternative was studied because the latter are known to have excellent space-time localization properties with significant advantages in data handling capability. The study carried out here showed that wavelet basis functions can be used to estimate accurately in an analytical fashion the diffusion term (with the higher order derivative) using connection coefficients evaluated from wavelet coefficients by suitably combining with the Galerkin multiple shooting formalism. Furthermore, the use of wavelet basis functions affords studying long time evolution of spatiotemporal
dynamics, its synchronization properties and multi-time scale features in a fashion much easier than empirical basis functions. The resulting advantages in estimating system parameters when only some variables are monitored using the devised multiple shooting algorithm for spatiotemporal systems has been clearly brought out. Online estimates of parameters from processes is an important goal in realizing practical applications, that would facilitate accurate model building from data, along with development of control and optimization strategies for highly complex dynamics.