Chapter 5

Summary

In this thesis spatio-temporal data from computer simulations of two reaction-diffusion systems were examined. The first system investigated was a generic model for the heterostructure hot-electron diode driven in a circuit under current-controlled conditions. The spatio-temporal data sets for this system are characterised by perfect spatial coherence. The absence of transient behavior could be confirmed by the proper orthogonal decomposition. The empirical modes found are very similar for periodic and chaotic behavior. As indicated by the singular values few of the modes suffice to describe almost all the variance of the dynamics. The first and the second mode could be assigned to the spiking and the nearly homogeneous oscillation between the spikes, respectively. For this system the attractor reconstructions from the global data, from mode amplitudes and from different spatial locations were made. It was shown that for spatial coherent dynamics equivalent information can be drawn from these different data sets. Even though a very long run of transient-free data was available, the estimation of the attractor dimension for the temporal chaotic data with a nearest-neighbor procedure lead to values smaller than two. The Lyapunov exponents computed from the same data sets also have to be considered as meaningless, because they lead to Kaplan-Yorke dimension smaller than two. The maximum map revealed that the dynamics is very inhomogeneous, phases of strong error amplification alternate with phases where deviations are almost wiped out. The corresponding parts in the attractor were identified. The inhomogeneity of the attractor is the reason that the values obtained for attractor dimension and Lyapunov exponents are spurious. This underlines the fact that even for purely deterministic systems where it is known that low-dimensional chaos is present one must not expect numerical procedures for the estimation of dimensions or Lyapunov exponents from time series data to give meaningful results.

The second system examined was a three-variable model for the heterogeneous catalytic oxidation of carbon monoxide on a platinum surface. It was found that for the data sets were due to transient or weakly turbulent behavior the mathematical premise of spatial coherence is not strictly satisfied valuable information can be drawn from the proper orthogonal decomposition. By this method it is possible to identify non stationary portions in the spatio-temporal data that cannot be found otherwise. It was found that the singular values corresponding to the mode amplitudes describing the non stationary behavior even give a quantitative measure for the amount of transient or turbulence present. This information can neither be drawn from the global data nor directly be read off the spatio-temporal data. Linear predictions using autoregressive models were made for different amplitude contours. The accuracy of these predictions indicated that the examined data are dominated by linear correlations. The estimation of the Lyapunov exponents again led to spurious values. Using delay coordinates the toroidal structure of the underlying attractors could be revealed. The attractor dimensions for the data sets were determined. Thereby it was found that the non-periodic data sets correspond to low-dimensional chaos.

For both systems the use of classical methods of data analysis like Fourier transform, autocorrelation function and histogram turned out to be essential to understand the results of the further analysis.

A new method that allows to determine wether an autoregressive model is stable without using the roots of the characteristic polynomial was introduced. This is achieved by transforming the autoregressive model into a moving-average model of infinite order. For a stable model the same procedure allows to compute the variance to high accuracy.

A program that combines most of the methods of data analysis used in this thesis was written in C++ (see Appendix C). Apart from the numerical procedures a certain emphasis was laid upon data visualization and interactivity. The source code is available from the author.