CELLULAR PATTERN FORMATION AND NOISE IN O(2) SYMMETRIC SYSTEMS

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Scott Arthur Gasner
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The Undersigned Faculty Committee Approves the
Dissertation of Scott Arthur Gasner:

CELLULAR PATTERN FORMATION AND NOISE IN O(2) SYMMETRIC SYSTEMS

Peter Blomgren, Chair
Department of Mathematics and Statistics

Antonio Palacios
Department of Mathematics and Statistics

Thomas Impelluso
Department of Mechanical Engineering

Alpan Raval
Department of Mathematics, Claremont Graduate University

Ali Nadim
Department of Mathematics, Claremont Graduate University

Approval Date
DEDICATION

Dedicated to
my wife Kelly Beachell Gasner,
my family, Larry Gasner, Lovice Gasner,
Glenn Gasner, Paul Gasner, and Emily Gasner,
and my best friend, Rob Carey,
for their support.
ABSTRACT OF THE THESIS

CELLULAR PATTERN FORMATION AND NOISE IN O(2) SYMMETRIC SYSTEMS

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Scott Arthur Gasner

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Cellular Pattern Formation occurs in numerous and varied physical systems, linked by their dynamics and symmetry properties. The characteristics of these systems can be described mathematically through symmetry breaking pattern formation. While focusing on the study of premixed laminar flame fronts, this dissertation seeks to provide insight across the study of cellular pattern formation in O(2) symmetric systems through the discovery of two robust new numerical solvers applied to the Kuramoto-Sivanshinsky Equation solved over a circular domain; a system for which there has been physical experimentation [31].

The deterministic solver improves on the prior best effort by avoiding linearizations and solving the fully nonlinear problem. Its success is shown through both analytical and practical methods. The resulting simulations can be run for long periods of time, even in the presence of complex and dynamic patterns. Bifurcation analysis is performed to provide support through comparisons to the physical experimentation. The resulting simulations provide a basis through with Birkhoff Normal Form equations are derived to offer other studies of cellular pattern formation in O(2) symmetric systems the benefit of our findings.

The additive noise solver provides another step towards simulating the physical experiments. Adjustments to the solver again allow for long simulations to be generated in the presence of complex and dynamic patterns. Most compelling is the fact that the results of the solver are dominated by dynamic states, a critical difference between the experience from the physical experiments versus deterministic simulations. The solver allows for the simulation of two dimensional intermittent flame patterns, including heteroclinic connections that have been observed in the physical experiments, but never before simulated using the Kuramoto-Sivanshinsky Equation. Normal form analysis provides a basis to show agreement to the physical observations. Additionally an intermittent direction switching rotation is simulated, and shown to exist in the normal form equations. The study of Complex systems provides the basis for the identification of the pattern as a noisy traveling wave.
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CHAPTER 1
INTRODUCTION

Cellular Pattern Formation is a physical phenomenon that has been studied for decades. It occurs in chemical, biological, and purely physical systems, driven through an activator-inhibitor mechanism first described by Turing [121]. The appearance of a cellular pattern is driven by symmetry breaking bifurcations in which the symmetry of the system plays a primary role in determining the family of patterns that can be observed. It is the asymmetry of the system, however, that determines the final selection from that family. Additionally, the omnipresence of noise in physical systems provides asymmetry and persistent perturbation, and must be considered in order to gain a complete view of a cellular pattern forming system using mathematical simulations.

Specific to this dissertation is the study of laminar flame fronts. Premixed gases burn irregularly, which can lead to cellular flame patterns [43]. When the gases are confined to circular domains, the cells become organized in stationary and nonstationary concentric rings. Stationary patterns are steady states with petal-like structures and well defined spatial symmetries. Nonstationary patterns are dynamic states that change continuously in space and time. The cells move either individually or collectively within the ring structure. The global dynamics could be as simple as a uniformly rotating cell or more complicated as an aggregation of cells moving chaotically [46]. An individual pattern, either stationary or nonstationary, is selected by the system based on control parameters such as type of fuel, pressure, flow rate and fuel-to-oxidizer ratio. Analysis of observed states have described the behavior of certain dynamic patterns including hopping states [92] and intermittent states [116]. The analysis was based solely on experimental data through the use of the Proper Orthogonal Decomposition, Marginal Stability Curves, and Passage Time distributions.
Gregory Sivashinsky used the exact equations for the combustion of premixed gasses to derive his famous model, the Kuramoto-Sivashinsky Equation [71, 107]. This equation provided the mathematical community with a precise nonlinear system to use in analyzing cellular pattern formation in laminar flame fronts. However, a comparative analysis against computer-simulated states was precluded by the lack of a reliable truly nonlinear two-dimensional numerical solver to integrate the equation. The prior best effort used Distributed Approximating Functionals (DAFs) to accurately solve for spatial derivatives, but relied on linearizations in time. The result was a scheme in which small nonlinear errors lead to divergence when simulating complex patterns, or covering time frames greater than a few hundred frames.

With this dissertation, we report two new robust numerical integration schemes that generate thousands of time frames, even when simulating complex patterns. In addition, the new schemes solve the fully nonlinear system in both space and time dimensions. This provides improved accuracy, which is displayed through the ability to produce simulations that better resemble the actual laboratory experiments, as well as the first simulations of several phenomena never simulated before. These schemes open the door to a deeper analysis of cellular pattern formation in $O(2)$ symmetric systems.

While much of parameter space remains open for analysis, the deterministic nonlinear numerical integrator for the Kuramoto-Sivanshinsky Equation has already produced an example of a 2 dimensional hopping state. The actual hopping state is a single-ring state made up of three cells, found in a very small region of parameter space bounded by two stationary patterns, one with three cells and one with four. A POD analysis reveals the emergence of a spatio-temporal pattern whose temporal characteristics are in good agreement, up to a few subtle differences in spatial behavior, with those of experimental states. This simulation confirms prior results [92] and provides the foundation for further analysis. Unlike other dynamic states, the hopping state results from the interaction of three steady-state modes, ones for which Birkhoff Normal form equations
have not existed. Our analysis proceeds through symmetry-based arguments to derive the normal form equations governing the existence of hopping patterns. The result includes conditions for the existence and stability of hopping states.

Through the additive noise nonlinear numerical integrator we seek to model thermal fluctuations occurring in premixed gas flames. The robustness of the solver provides again for many thousands of time steps to be taken, even in the presence of complex patterns. A preliminary investigation of parameter space has already produced simulations of several 2 dimensional intermittent states. A single cell intermittent direction switching rotation, and an intermittent one-two heteroclinic state are found between a one cell stationary state and a two cell stationary state. Intermittency has been observed in laboratory experiments, including a one-two intermittent state found in the center of 8 stationary cells [44]. Other experimental observations of intermittency include more complex patterns, which are also within the parameter ranges handled by our solver. Analysis of the behavior of the one-two intermittent state shows that the simulated state exhibits a passage time distribution that is in good agreement with the experimentally observed states. The single cell direction switching rotation is shown to exist in the normal form equations for the system. A statistical distribution of amplitudes displays the agreement with current theory regarding pitchfork bifurcations in the presence of additive noise. In all cases we discuss the analysis in detail in this dissertation.

The dissertation is organized as follows. In Chapter 2 we review the history of Cellular Pattern Formation with an emphasis on those involving \(O(2)\) symmetry. We also introduce the Kuramoto-Sivanshinsky equation and discuss the history of its derivation. A brief statement regarding the combustion experiment that is the physical basis of this study is also given. Interested readers will find a more complete review of the findings of physical experiments in Appendix A. Chapter 3 contains our implementation of the deterministic fully nonlinear integration scheme that provided the preliminary results. A companion to this chapter is found in appendix B where we describe the numerical methods implemented in
this study. Templates for the Crank-Nicolson Method, Distributed Approximating Functionals, BiCGStab, and Nonlinear Newtons Method are given. In Chapter 4 we describe the POD approach, Marginal Stability Curves, and Normal Form Equations as they relate to the simulation of the three cell hopping state. Since the hopping state discovered in this study is novel, we use it to derive new normal form equations for use by researchers studying other systems. A companion to this chapter is found in appendix C where we elucidate the Proper Orthogonal Decomposition (POD), Method of Snapshots, stability analysis, bifurcation analysis, and normal form equations in relation to the interaction between single cell and a two cell steady states. Chapter 5 contains the description and results of the Additive Noise study. First we present a basic review of the physical phenomena modeled by a Langevin Formulation of the Kuramoto-Sivanshinsky Equation. Then we describe the Nonlinear Stochastic Integration Scheme implemented, and provide a Code Flow Diagram. We describe the new intermittent cellular patterns found in the study, and decompose these new patterns to reveal their characteristics. We then show the agreement between the direction switching single cell rotation and single cell unsteady state to a Langevin formulation of the normal form equations. Next we then show the agreement between the simulated one-two heteroclinic state and the passage time distributions of the normal form equations. The normal form equations have been shown in other work [116] to well describe the cellular flame experiments at the base of our study. Chapter 6 contains some conclusions from the study and suggests a variety of further research.
CHAPTER 2
BACKGROUND

The first description of cellular flames occurred in a paper entitled "The structure and chemistry of flames" by Smithells and Ingle in 1892 [114]. The two authors were reporting on their observations of bunsen burner flames. The report concerns the ability to separate flame fronts from distinct reactions occurring during the combustion of a premixed gas. With a modified bunsen burner, they were able to discern two conical flame fronts, one inside of the other, while burning benzene mixed with air. They noted that when the benzene was supplied in excess, the inner cone grew until it was very tall, and eventually broke through the outer cone. When the benzene supply was limited the upper cone vanished completely, and the inner cone grew bright and hot. For a certain supply of benzene, the two observed a polyhedral flame front, stating “The inner cone presents a peculiar appearance. It is divided into several (usually five or six) petal-like segments, which often revolve with great rapidity round a vertical axis.”

Figure 2.1. The bunsen flame separation experiment by Smithells and Ingle in 1891 [114].
Polyhedral flames became the focus of a paper by Smith and Pickering in 1928 [113], who were also experimenting with a mixture of combustible gas and air on a bunsen burner. They published photographs of polyhedral flames observed in a propane-air mixture. Early images of cellular flames produced in large number on a circular burner can be found in a book entitled *Non-steady flame propagation* edited by George Markstein and published in 1964 [79].

In 1977 Gregory I. Sivashinsky derived the first nonlinear equation for a laminar flame front [107]. At the same time, another scientist named Yoshiki Kuramoto developed a similar equation while modeling diffusion-induced chaos [71] in a study of the Belousov-Zhabotinskii reaction in three dimensions [58]. Their simultaneous discovery is known as the *Kuramoto-Sivashinsky Equation*. Sivashinsky’s earlier work provided the support for his derivation of the Kuramoto-Sivanshinsky equation. Some of his first work on flames produced on a circular burner involved bunsen burners [105]. In fact, his equation for the reaction rate intensity from this paper proved necessary for the derivation in 1977. An earlier paper from 1977 laid the groundwork for his nonlinear analysis by describing the diffusional-thermal theory of cellular flames [106]. A companion paper to his derivation contained some early numerical simulations performed in a single dimension [84]. The constant density approximation allows for the separation between hydrodynamic and diffusional-thermal instabilities, and lead to further models in a paper from 1979 [82]. As an expansion on the prior one dimensional simulations, some basic two dimensional patterns were simulated in 1980 [80]. A study furthering the understanding of cellular flame fronts considered the prior derivation under conditions of stoichiometry [108], and in the end provides an alternative derivation of the Kuramoto-Sivanshinsky. Rotating states are shown to be a possible result of a bifurcation of a planar wave in a paper written in 1981 [109]. A linear analysis of non adiabatic flames was shown to describe cellular flames in another work by the great man in the same year [111]. His later work on flame fronts dealt with modeling the three dimensional flame fronts of flame balls; balls of flammable gas that are ignited by
a spark [110]. This work closes the loop between Sivashinsky’s two dimensional models and the spherical flame study performed by Istratov and Librovich [60] that gave tremendous support to his derivation of the Kuramoto-Sivanshinsky equation.

Sivashinsky’s theory showed that diffusion-induced chaos was a viable theory to describe flame dynamics. An immediate and large effort was put forward by the mathematical research community to explore this possibility. Major scientists and studies are described here for the interested reader. Studies have investigated the bifurcation phenomena in burner-stabilized premixed flames [78]; conductive interactions of wrinkled flames with cold flat burners [64]; stability of the porous plug burner flame [15]; viscoelastic behavior of cellular solutions to the Kuramoto-Sivashinsky model [36]; approximate inertial manifolds for the Kuramoto-Sivashinsky equation [63]; bifurcations and pattern formation in the regularized Kuramoto-Sivashinsky equation [17]; nonlinear dynamics of cellular flames [8]; and the transition to spatiotemporal chaos in the damped Kuramoto-Sivashinsky equation [32] among many other topics.

While much work has been done in a single spatial dimension, few have numerically simulated a two dimensional flame front. While one dimension may capture the general behaviors of the patterns, they cannot distinguish the finer details. For instance, a rotation cannot be observed in one dimension. This dissertation seeks to further the understanding of chaos and pattern formation at the basis of cellular flame dynamics; with the grander goal of providing insight into other cellular pattern forming systems with $\text{O}(2)$ symmetry.

2.1 Cellular Pattern Formation in Science

Pattern formation is a study born through simple observations of nature. From patterns in shells, to branching in trees, and the shape of pine cones, there is no doubt that nature exhibits patterns. These types of observations interested the earliest philosophers whose quotes on the matter have survived to the modern age.

Pythagoras - *Numbers rule the Universe.*

Plato - *God ever geometrizes.*
The classic task is to identify the mechanisms with which these patterns are formed.

### 2.1.1 Symmetry Breaking Bifurcation

The first reference to the symmetry of the system having a significant effect in the outcome of a physical process comes from Pierre Curie, the husband of Marie Curie who discovered Radium\[26, 85\]. In 1894, while studying electromagnetism, Pierre Curie published what is now known as the Curie Principle of Symmetry and Asymmetry. It can be written in three parts,

1. *If certain causes yield certain effects, then the symmetry of the causes appear in the symmetry of the effects.*
2. *If certain effects manifest a certain asymmetry, then this asymmetry will be reflected in the causes.*
3. *The converse to the two previous propositions is not true, in that the effects may have a higher symmetry than the causes which generate these effects.*

Thus Curie determined a causal relationship where the results of an interaction between causes would have the same or higher symmetry than the causes themselves.

Curie’s Principle appears to be in contradiction to what has been observed since, especially through nonlinear instabilities, where the results commonly have reduced symmetry as compared to their causes. The best known example contradicting Curie comes from a book published in 1942 titled *On Growth and Form* by D’Arcy Thompson [119]. It contains the well known image of a splash crown created in milk, see FIG. 2.2. The image is well known as it has captured the entire process of a loss in symmetry. The initial milk droplet is, except for the effects of gravity and shear forces, essentially spherical, containing circular symmetry in 3 dimensions. Upon impact with the surface of the milk, the result is a splash which has 24 points. Each of these points has thrown off a minute droplet, or is in the process of throwing one off. Assuming that the slight differences between the points of
the crown are caused by imperfections in the experiment, one still is left with a result that has less than circular symmetry.

![Image](image.jpg)

**Figure 2.2.** 24 point splash crown in milk published by D'Arcy Thompson [119].

This viewpoint was championed by Stewart and Golubitsky in 1992 [115] who described the case where a symmetric system begins to exhibit less symmetry, calling it a *Symmetry Breaking Bifurcation*. They point out that symmetry breaking does not necessarily disprove the Curie Principle if viewed from a certain point of view. Citing the milk droplet example, they indicate that mathematically the crown could have formed at any rotation, a fact made obvious by considering that the observers point of view is not mandated by the system. Due to the circular symmetry of the system, a priori the mathematician can only predict the shape (pattern) of the crown, not its orientation.

Of course, in reality a single solution must occur. This reduction to a single solution seems to be driven by imperfections in the symmetry. For instance, the droplet may not be perfectly spherical, it may have a tiny dimple of its surface. Even smaller imperfections exist, such as the thermal fluctuations in the atoms of the milk that will almost definitely not be perfectly spherically symmetric within the droplet. These asymmetries will effect the splash, and through them a single case from the family of splashes will result.
Curie's Principle reflected the observation that the symmetries in the result of an interaction will maintain the symmetries of the causes, but also that asymmetries of the results come from asymmetries of the causes. The issue is scale. The spherical symmetry comes from an observation of the entire droplet. The asymmetric imperfections from small scale regions within the droplet. Yet in the resulting splash, the small scale imperfections have a large scale effect, determining the orientation of the splash. So Curie was right; the only issue is that objects in the real world are never perfectly symmetric.

2.1.2 O(2) Symmetry

Of particular interest to this dissertation is the two dimensional orthogonal symmetry group, called the O(2) symmetry group. By definition, this group consists of all $2 \times 2$ matrices $A$ satisfying

$$AA^T = I_2,$$

(2.1)

where the superscript $T$ symbolizes the transpose [41, 89]. This group is sometimes called the circle group, because matrices which are elements of O(2) are invariant to rotation and reflection. Take $\Gamma$ to symbolize the O(2) symmetry group, and $\gamma \in \Gamma$. Also let us define the identity matrix $I$, the reflections matrix (a.k.a. the flip matrix) $R_f$, and the rotations matrix $R_\phi$ as follows:

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R_f = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R_\phi = \begin{bmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{bmatrix}, \quad \phi \in [0, 2\pi).$$

(2.2)

These matrices describe transformations which are $\Gamma$ invariant, i.e.

$$II\Gamma = \Gamma \quad R_f \Gamma = \Gamma \quad R_\phi \Gamma = \Gamma$$

(2.3)

Also, the matrices $R_f$, and $R_\phi$ are generators of $\Gamma$. We know that the identity $I$ is an element of every group, and that the elements of every group can be formed by a finite combination of their generators. Therefore we can describe every $\gamma \in \Gamma$ through some combination of $I, R_f, \text{ and } R_\phi$. 
The two dimensional special orthogonal symmetry group, called $\text{SO}(2)$, is a subgroup of $\text{O}(2)$ in that it consists of all $A \in \Gamma$ such that $\det A = 1$. It is sometimes called the 2 dimensional rotation group as it consists of all of the planar rotations described by $R_\phi$. In fact, $R_\phi$ is a generator for $\text{SO}(2)$. It can be seen that the identity matrix $I$ can be obtained by setting $\phi = 0$. Notice that the flip $R_f$ is not a generator for $\text{SO}(2)$, which denotes that reflections are not a property of this group.

The dihedral group, called $D_n$, order $2n$, is the symmetry group of the regular $n$-gon. This group can be described as the group of $2 \times 2$ matrices generated by the flip $R_f$, and a fixed rotations matrix $R_{2\pi/n}$, which is the same as $R_\phi$ except that the value of $\phi$ has been fixed such that $\phi = \frac{2\pi}{n}$. Notice that each group $D_n$ is also a subgroup of $\text{O}(2)$.

$\text{O}(2)$ Symmetry has been observed experimentally in systems involving ferromagnetics as in the site frustrated Heisenberg model [9]; optics as in the light beam emitted by a photorefractive oscillator [33], biology as in elongated particles [38]. It has been theorized to exist in systems involving black holes in ten to eleven dimensions [27]; unstable electrostatic waves in an unmagnetized Vlasov plasma [24]; overlapping instanton pairs [95], filament dynamics involving solitons [14].

### 2.1.3 Cellular Pattern Formation

The word “cellular” originally referred to cells within living tissue. As early as the 17th century, the patterns of cells within living tissue were observed to be similar in structure across many different tissues, as well as to many structural patterns across other disciplines [15]. Biologists noted the similarities to patterns of different scales, including territorial patterns [30, 21]. Geologists noted the cellular structure of rocks created in lava flows [18]. More recently this type of structure was found in material science, they appear in mud cracking patterns, in ceramics and minerals [1], polycrystalline metals, soap suds, bubbles in lipid monolayers, bubbles in fluidization and solidification processes, and magnetic bubbles [39], in vibrated granular systems [120], and in honey combs [67, 30]. Numerous other examples can be found in the thesis by Jiang [62]. These sorts of cellular pattern
formation result through a competition between a minimization process, for instance surface tension, and some geometric constraint, for instance an equilibrium pressure within some boundary. In one example provided by Hildebrandt and Tromba a comparison is made between the structure of a dragonfly wing and soap bubbles within a wire frame [51]. It can be observed that the soap bubbles well approximate the living cells that formed the wing, see FIG. 2.3.

![Figure 2.3. A dragonfly wing (top) is approximated by soap bubbles (bottom) in a wire frame. The wire appears as dark lines. Note that the bubbles meet each other at 120° angles and meet the wire frame at 90° angles. Reprinted from the work of Hildebrandt and Tromba [51].](image)

Another sort of cellular pattern formation, involving reaction-diffusion systems, was first suggested by Alan M. Turing in 1952 [121]. He realized that cellular pattern formation in these systems requires a slowly diffusing activator and a more abundant inhibitor. He was studying morphogenesis, or the process of growth in an embryo, and identified that once an instability grows, it could appear in a ring with peaks equally spaced due to a characteristic wave length as either standing or traveling waves. He also noted that minute asymmetries allow for bifurcation, stating that perfectly spherical blastula would remain perfectly spherical forever and certainly not grow into a horse.

This type of cellular pattern formation has been observed in many physical systems including Modulated Taylor-Couette Flow, which is the flow between two concentric
Figure 2.4. Near-field images of a 6µm Vertical cavity surface emitting laser (VCSEL) pump currents as indicated to the left of each row. Column headers indicate the polarization of the near-fields. Reprinted from the work of Degen et al. [28].

cylinders [74]; three-dimensional Rayleigh-Bénard convection [4, 99, 101]; von Kármán swirling flow, which is flow between to spinning disks in a stationary cylinder [87]; chemical systems including reactions in gel [88]; laser dynamics such as multi-transverse-mode near-fields of circular vertical cavity surface emitting lasers (VCSELs) [28], see FIG. 2.4; photospheric granulation [16]; and the variability in number of cotyledons formed by conifer embryos [50], see FIG. 2.5 and FIG. 2.6.
Figure 2.5. Images of Larix × leptoeuropaea somatic embryos taken using a Scanning Electron Microscope display a varying number of cotyledons, equal to 1, 2, 3, 4, 5, 6, 8 respectively. These images are reprinted from Harrison and von Aderkas [50].

Figure 2.6. Image of Larix × leptoeuropaea somatic embryo exhibiting a growth abnormality, called a crater, that usually fails to produce any cotyledons. This image is reprinted from Harrison and von Aderkas [50].

Understanding the mechanisms that govern the spatial and temporal evolution of cellular patterns, and their response to noise, is important because such knowledge may be applied broadly across the sciences. It occurs during morphogenesis, and therefore can be applied to biology, for instance, for the purpose of effecting the number of stems produced by a single seed, or perhaps learning more about growth abnormalities in a fetus. It occurs in fluid flows, and may be useful in designing new mixing devices. It occurs in materials and could lead, for instance, to novel designs and developments of new materials. It also occurs
in laser dynamics, combustion and other chemical systems, for which the list of possible applications are numerous.

2.2 The Kuramoto - Sivashinsky Equation

When a premixed gas is burning, the rate of the reaction \(W\) is proportional to the temperature \(T\). This phenomenon, known as Arrhenius conditions, is common to virtually all chemical dynamics. The rate of increase is governed by the activation energy of the mixture \(E\), and the universal gas constant \(R\).

\[
W \sim \exp\left(-\frac{E}{RT}\right).
\]  

Once a volume of the fuel and oxygen mixture is ignited, an exothermic reaction begins. The burning gas causes the temperature of the surrounding gas to increase to the point of combustion induction causing the reaction to spread throughout the available gas. This self propagating combustion reaction wave is commonly referred to as a “premixed gas flame.”

A gas burner allows the stream of premixed combustion gases to pass through a burner aperture at a steady rate. Consider the case of a well-formed flame front, where the transitionary period of its formation has been completed. There is oncoming gas flowing downstream. This gas is composed of combustion reactants, and perhaps an inert diluent which carries the reactants, but does not take part in the reaction. As the flame propagates in free space, we may consider the rate of reaction as being proportional to the temperature alone. The downstream gas is still too cool to burn, and gradually heats up as it approaches the flame front. When the gas reaches a critical temperature within the flame, it rapidly combusts, propagating the reaction wave to the premixed gas immediately following. The process of combustion is very quick and the resulting burned gas passes out past the flame, exhausted of the reactant.

The thermal thickness of the flame \(\ell_{th}\) is defined as \(D_{th}/U_u\) where \(D_{th}\) is the thermal diffusivity of the mixture, and \(U_u\) is the propagation speed of the flame relative to
the unburned gas

\[ U_u = \sqrt{\frac{2D_{th}}{T_b - T_u}} \int_{T_u}^{T_b} W(C, T) \, dT, \]  

(2.5)

\( T_u \) is the temperature of the unburned cold gas mixture, and \( T_b \) is the maximum temperature reached during the reaction, usually many fold higher than \( T_u \). The majority of the burning occurs in a more narrow region \( \ell_r \sim (RT_b/E)\ell_{th} \), where the temperature is the highest, which is commonly about 1/20 of the thermal thickness of the flame. For example, a rapidly burning mixture such as \((2H_2 + O_2)\) would have \( U_u \approx 10m/s \) and \( \ell_{th} \approx 0.0005cm \). A slowly burning mixture, such as \((6\%CH_4 + air)\) would have \( U_u \approx 5cm/s \) and \( \ell_{th} \approx 0.05cm \) [110].

It is possible for a flame front to hold the form of a single steady plane. In order for this to occur the flame must be under small disturbances. Many flames are known to behave this way under controlled conditions. This simple structure can be described mathematically using only one dimension, which was done in the 1960s [124]. However, for combustion over wide apertures, the flame commonly breaks up into separate cells \( \sim 1 \text{ cm} \) to \( 10 \text{ cm} \) in size. The cells that appear on the surface of a flame have a characteristic dimension underlying their three dimensional structure. The magnitude of this characteristic dimension depends on the mixture being burned. Thus as the radius of the flame grows, so do the number of cells appearing on the flame front [110].

The flame front is an internal boundary layer that is often visible between the unburned and burned gas. Interestingly, if we were to investigate a combustion reaction at the asymptotic limit of large activation energy, the flame front would shrink in depth until it was a two dimensional surface. This represents a significant simplification, allowing for a complete investigation of a three dimensional reaction region to be performed through an analysis of a two dimensional reactive front. Due to Arrhenius kinetics a two dimensional reactive front would actually be the case for a combustion requiring an infinitely large activation energy [77].
Since all chaotic systems exhibit a sensitive dependence on initial conditions, it is almost always impossible to determine the exact outcome of any experiment. Instead the experimentalist usually observes the system approaching some steady state that can be described as a pattern. In these cases, the study of pattern formation provides the most complete method of prediction for the experimentalist. It is natural for the mathematician to analyze the pattern formation mechanism through a study in the same number of dimensions in which the experimentalist is working. Analysis performed through the integration of the Kuramoto-Sivanshinsky in two dimensions allows for the study of dynamic patterns that in a single dimension could only be shown to be stable.

2.2.1 Cellular Flame Fronts

There are two sources of instability for premixed gas flame fronts. One is due to thermal expansion, the other due to thermo-diffusive instability. Thermal expansion is the process that leads to the formation of wrinkles on a premixed gas flame front. It was described as early as 1944 by Landau [72], and later in 1964 by experimentalist G.H. Markstein [79] whose work also included some of the first images of cellular flames. Markstein found that wrinkles, distinct from cells, were formed on a flame front by external forces. For example if the flame front passed through a wire mesh, a regular pattern of wrinkles would result on the flame front. If the flame front were to grow in size, the wrinkles would remain, and grow in size. The wrinkles will deepen and remain in the same number. The presence of wrinkles was shown to increase the mean propagation velocity. It is important to note that wrinkles do not appear on the flame front in the absence of external perturbation. This instability alone is not known to lead to self-turbulence of premixed gas flames. It is considered a hydrodynamic effect.

Istratov and Librovich published a comprehensive study concerning the stability of spherical premixed gas flames in 1969 [60]. The premixed gas spherical flame has the distinct advantage over planar flames in that it has no boundary effects. The study described three distinct regions of instability, each occupying a certain range of the mean
propagation velocity. These regions separate the effects of thermal expansion from those of thermo-diffusive instabilities. For low mean propagation velocity the flame front was laminar, unless an external force caused wrinkles due to thermal expansion. Low mean propagation speed flames are also quite small, and therefore immune to large wavelength perturbation. As the mean propagation speed is increased, the flame radius also increases. As it passes beyond some critical value, uniformly distributed weak protuberances appear, i.e. flame cells. In this region, as the radius of the flame is increased, the number of cells also increases, although the characteristic dimension of cells remains constant. It is interesting to note that the wrinkles on the flame front are maintained throughout this region. As the radius is further increased beyond another critical value, self-turbulence sets in, and all structure is lost. In this region there is a persistent and random splitting and merging of cells. This behavior is sometimes referred to as a dynamic pulsating cellular flame. It is in this region that the wrinkles on the flame front are destroyed. As the radius is further increased, the flame forms a detonation wave.

2.2.2 The Discovery and Evolution of the Kuramoto-Sivashinsky Equation

In Gregory Sivashinsky’s seminal work [106], the flame model described by Istratov and Librovich [59] provided the fundamental equations describing diffusion, heat conduction, continuity, momentum, and the dynamic incompressibility condition. These are the exact equations used for the nonlinear analysis whose result is the Kuramoto-Sivanshinsky equation. Other models are also used in the derivation, including that of Landau [72], Zel’dovich et al. [125], and Barenblatt et al [5]. In order to provide an equation that could be used to investigate cellular flames, Sivashinsky knew that a nonlinear equation would be needed.

In that derivation, Sivashinsky tried to qualitatively describe the forces driving the shape of the flame front. He found that the conduction of heat has a stabilizing effect on flames. The troughs of a curved flame are hotter, causing them to burn toward the supply
of fresh reactant more quickly than the cooler crests of the flame front. If the rate of conduction of the heat were high it would tend to smooth out these temperature differences stabilizing the structure into a more planar shape [106].

Diffusion, on the other hand, has a destabilizing effect on flames. When the rate of diffusion is high, the hotter troughs will encounter a greater amount of fresh reactant. This will allow them to grow hotter yet, pulling them deeper toward the source of fresh gas. When the molecular diffusivity of the limiting reactant is sufficiently greater than the thermal diffusivity of the mixture, a planar flame front would be unstable [106].

It is interesting to note that the temperature of the flame at any point is directly correlated to the luminescence at that point. Thus the hotter troughs will also be brighter, while the cooler crests would appear darker. This phenomenon allows the experimentalist to observe the evolving temperatures within a flame based on its appearance [94].

The hydrodynamics of the underlying mixture will directly effect the behavior of the flame front, and can produce corrugated and cellular flame front structures [35]. This aspect of flame dynamics is uncorrelated to the behavior caused by the diffusional-thermal properties of the mixture, and should be considered separately. It can be shown that the cellular structure of flames can be described without introducing the effects of the hydrodynamics of the mixture. It should be noted, though, that the hydrodynamic effects also can lead to cellular flames as shown by Markstein [79]; where perturbations to the burner caused cells to appear on the flame front. If we assume that the mixture is motionless in the initial condition, then it can be assumed that it is motionless throughout the experiment as the flame passes through it. In assuming this, we also assume that the density of the gas is constant. Then the thermal perturbations cannot be transformed into hydrodynamic perturbations, separating the problem of combustion from the problem of hydrodynamics [106].

A perturbation analysis of laminar flames shows that, for the general case, a plane flame front may be unstable to long-wave disturbances (especially when large in scale [59]).
although it is always stable to short-wave disturbances [110]. The effect of a long-wave disturbance was described by Barenblatt in 1962 [5] through the dispersion relation:

$$\sigma = D_{th} \left[ \frac{1}{2} \beta (1 - Le) - 1 \right] k^2. \quad (2.6)$$

Here, $\beta = E(T_b - T_u) / RT_b^2$ describes the rate of the reaction given the difference in temperature between the burned gas and the unburned cold gas mixture. $D_{mol}$ is the diffusivity of the limiting reactant, which is the reactant that is totally consumed by the reaction. $D_{th}$ is the thermal diffusivity of the mixture. $Le = D_{th} / D_{mol}$ is the Lewis number of the limiting reactant which is assumed to be strongly deficient. $\sigma$ is the rate-of-instability parameter and quantifies the instability caused by the perturbation. $k$ is the wave vector of the perturbation to the flame front $F \sim \exp(\sigma t + i k \cdot x)$ [110]. It is clear that if the diffusivity of the limiting component ($D_{mol}$) is sufficiently larger than the diffusivity of the mixture ($D_{th}$), the value of the lewis number ($Le$) would be small enough that the flame front would be unstable to long-wave perturbations.

Sivashinsky noted [106] that Barenblatt's Eq. 2.6 did not account for the stability of a planar flame front to short-wave perturbations. He therefore added a nonlinear term to improve the model. The following was derived for systems where $Le \approx Le_c$:

$$\sigma = D_{th} \left[ \frac{1}{2} \beta (1 - Le) - 1 \right] k^2 - 4 D_{th} \ell_{th}^2 k^4. \quad (2.7)$$

Thus a system is stable when the diffusivity of the limiting reactant is less than a critical value ($Le > Le_c = 1 - \frac{2}{\beta}$). When $Le < Le_c$ some of the perturbations will have positive $\sigma$ and therefore positive amplification rates. Therefore there would exist a wavelength $\lambda_c$ which would dominate the shape of the flame front (maximum $\sigma$) and have the greatest effect on its shape [110].

This linear stability analysis with respect to the wavelengths of disturbances essentially represents a Fourier transform of the system. Since each disturbance is orthogonal to every other disturbance, they can be summed into the following linear
equation of the flame front [110]:

\[ F_t + D_{th} \left[ \frac{1}{2} \beta (1 - Le) - 1 \right] \nabla^2 F + 4D_{th} \ell_{th}^2 \nabla^4 F = 0. \]  

(2.8)

Now that we have described the behavior of the distortions to the flame front, it is important that we include terms describing the curvature of the unperturbed flame front given our assumptions. According to Sivashinsky, the radius of curvature of the flame front is much larger than the thermal thickness of the flame \( \ell_{th} \), then the propagation speed of the flame relative to the gas is constant and equal to \( U_b \). This characteristic is described by the eikonal equation:

\[ F_t = U_b (1 - \sqrt{1 + (\nabla F)^2}). \]  

(2.9)

When a system that is near the stability threshold \( Le \approx Le_c \), the gradient of the flame front should be small, and therefore \((\nabla F)^2 \ll 1\). Hence

\[ F_t + \frac{1}{2} U_b (\nabla F)^2 = 0. \]  

(2.10)

Combining this weakly nonlinear equation for the undisturbed flame front with the nonlinear equation for the disturbances to the flame front yields a model that fully describes the perturbed flame front [110]:

\[ F_t + \frac{1}{2} U_b (\nabla F)^2 + D_{th} \left[ \frac{1}{2} \beta (1 - Le) - 1 \right] \nabla^2 F + 4D_{th} \ell_{th}^2 \nabla^4 F = 0. \]  

(2.11)

This equation proved suitable for producing simulations of the expected distinct flame behaviors. Wrinkled, cellular, wrinkled cellular, and turbulent flame fronts were generated in a companion paper written with D. M. Michaelson [84]. The simulations were performed in one spatial dimension.

Sivashinsky acknowledged one hydrodynamic effect in later work [81]; that the heating of gas results in thermal expansion. It was noted that the gas expansion upstream of the flame front would resist the force of the flame front to travel upstream. This “buoyancy” would therefore have a stabilizing effect on the flame front. The stabilizing
force term, \( g(1 - \epsilon)/2U_b \) where \( \epsilon = \rho_b/\rho_u \), was added to the equation to account for this force. The following is a revised, non-dimensionalized version of the equation:

\[
\Phi_t + \frac{1}{2}(\nabla \Phi)^2 + \nabla^2 \Phi + 4\nabla^4 \Phi + G \Phi = 0.
\]

(2.12)

The symbol \( G \) is proportional to the reciprocal of the Froud number, and should stabilize the flame front completely when it is greater than 1/16. When \( G \) is near this stability threshold, the flame front should stabilize into a cellular structured steady state.

The Kolmogorov-Spiegel-Sivashinsky model is an adaptation of the Kuramoto-Sivashinsky model that adds a cubic nonlinear term to the equation. It is as follows:

\[
\partial_t \Phi + (\partial_x \Phi)^2 + \partial_x^2 \Phi + \partial_x^4 \Phi + \eta \Phi - \delta \partial_x(\partial_x \Phi)^3 = 0.
\]

(2.13)

It is believed that the addition of the cubic term leads to a shift in the threshold for the appearance of chaos, as well as a modification in the character of the transitions [25].

In 1986, Sivashinsky teamed with M. L. Frankel to expand on his prior work on the thermal diffusive theory of curved flames [34]. The work focuses on the form of the KS given as

\[
f_t + \frac{1}{2}f_x^2 + (\alpha - 1)f_{xx} + 4f_{xxx} = 0.
\]

(2.14)

The paper describes the derivation of a new form of the KS which is invariant to the choice of coordinate system. This would generalize the equation for use in more complicated hydrodynamics, including turbulent gas flow. Interestingly, the paper also includes a formula for the propagation velocity of the flame (\( V_n \)) in a direction normal to the flame surface,

\[
V_n = \frac{f_t}{\sqrt{1 + f_x^2}}.
\]

(2.15)

Since the propagation velocity of the flame was given by Sivashinsky [110] as the Ordering Parameter driving pattern dominance in premixed gas laminar flames, this formula opens the door to investigation of this tenet of flame dynamics. Further details are given in subsequent work [35]. A study involving the use of the flame front velocity as an ordering parameter for cellular flames is suggested in the conclusion of this dissertation, in Chapter 6.
2.3 Physical Experimentation

Modern combustion experiments were conducted by M. Gorman, among others, at the University of Houston [46]. A mixture of either isobutane and air, or propane and air, was burned on a circular porous plug burner within a low pressure (.3 to .5 atm) combustion chamber. The process allowed for control of the pressure, flow rate, and fuel to oxidizer ratio to within .1%. The surface of the flame that appeared was 5.62 cm in diameter and .5 mm thick.

Images of the flame front were recorded using a Dage-MTI charge coupled device camera, that was mounted vertically on top of the combustion chamber. A significant characteristic of flame fronts from premixed gasses, in terms of their spatiotemporal dynamics, is that the local temperature of the flame is exhibited in their chemiluminescence. The images were recorded on S-VHS video tape, and therefore have a pixel resolution of 640x480 taken at 1/30 sec intervals with a 7-bit dynamic range.

Changes in the experimental parameters (type of fuel, pressure, total flow, and equivalence ratio) resulted in different cellular patterns in the flame front. The hottest regions of the flame were also the brightest regions of the images. Gaps between the cells represent cusps and folds that extend up to 5 mm away from the surface of the burner. The simplest cellular pattern generated by the burner is a large single cell with $O(2)$ symmetry. As the system dynamics are altered through the parameters, the system was observed to bifurcate into more complex patterns through a sequence of symmetry breaking bifurcations. It was stated, however, that at any point in parameter space, the system may become disordered [31]. In order to observe most of the patterns seen, especially in the case of isobutane-air, the experimentalist would first find a well known ordered pattern, like the 6/1. Once the pattern was stable, the system parameters would be quickly changed to those in question. Thus the system was given an ordered state as an initial condition to help induce another stable pattern. Some of the patterns observed in these experiments were not
observed in the absence of this method to induce order. It should also be stated that some of the patterns were only observed for brief periods of time, as short as 1/30 of a second.

Figure 2.7. Examples of stationary ordered states observed in laboratory experiments, including the trivial state (a), a five cell (b), a six cell (c), a ring of eight cells surrounding a single cell (d), a ring of nine cells surrounding two cells (e), a ring of eleven cells surrounding three cells (f), a ring of twelve cells surrounding four cells (g), a ring of twelve cells surrounding five cells (h), a ring of thirteen cells surrounding six cells (i), a ring of thirteen cells surrounding six cells surrounding a single cell (j), a twenty-seven cell hexagonal lattice (k), a forty cell rhombic array (transient) (l). This image is reprinted from [43].
Results of the experimentation included the observance of many cellular flame states [44], see FIG. 2.7, which were categorized by their dynamics and number of cells. While the stationary flame states and rotations were observed as anticipated, many new dynamic patterns were observed for the first time. It was found that in the case of a multiple ring rotation, individual rings may co-rotate, rotating in the same direction, or counter-rotate, rotating in opposite directions [46], see Appendix Section A.2. Also, modulated rotations were observed in which a rotation is accompanied by fluctuations in velocity and/or cell shape and size. Examples include the ratcheting motion [42], described in Appendix Section A.4, and the hopping behavior [45] described in Appendix Section A.6. Intermittent patterns were observed and described as heteroclinic connections [44], see Appendix Section A.8. Pulsating flame states were observed in the extinction boundary [44], see Appendix Section A.7. A substantial review of the primary experimental results has been compiled in Appendix A.
2.3.1 The Naming Convention

Cellular flame patterns may occur in concentric rings. When this happens, the pattern is named by counting the number of cells in the outermost ring, and then in each concentric ring until the center is reached. Therefore a pattern with 15 cells on the outermost ring, 8 cells on the next concentric ring, and 2 on the innermost ring would be called a 15/8/2. To describe the dynamics of a spatiotemporal pattern, an alphabetic identifier is also included as follows:

\[
\begin{align*}
S &= \text{Stationary} \\
U &= \text{Unsteady} \\
R &= \text{Rotating} \\
CR &= \text{Counter Rotating} \\
H &= \text{Hopping} \\
I &= \text{Intermittent} \\
W &= \text{Ratcheting} \\
P &= \text{Pulsating}
\end{align*}
\]

When ratcheting occurs between two or more rings, the alphabetic descriptor is placed next to the number of cells in each ring. Thus a 12W/6W/1S describes a state where an outer ring of 12 cells, and a middle ring of 6 cells ratchet, while a central cell remains stationary [42]. Patterns described without an alphabetic descriptor are assumed to be stationary. For example, the 15/8/2 notation used in the prior paragraph suggests the cells to be stationary. In the case of intermittent dynamics, all of the the modes visited by the pattern are listed in it’s name. For instance, the 1-2I state is an intermittent state that visits both the 1S and 2S states.
CHAPTER 3
DETERMINISTIC NONLINEAR INTEGRATION
OF THE KURAMOTO-SIVASHINSKY EQUATION

The numerical scheme discussed in this dissertation is an extension of [126] which proposes a scheme for the time-integration of the Kuramoto-Sivanshinsky equation. The aforementioned scheme achieves highly accurate spatial derivatives using Distributed Approximating Functionals (DAFs), described in Section 3.1. It also uses linearizations when integrating in time. The proposed scheme solves the fully nonlinear problem, and is second order in time. Further, the new scheme, in which the time-integration is based on the Crank-Nicolson method [23], which was described in Appendix Section B.1, is unconditionally A-stable, thus producing finite solutions in all cases where the exact solution of the underlying equation produces finite solutions. The Crank-Nicolson scheme is coupled with an iterative Newton solver, described in Appendix Section B.3. It is the proper choice as they both can be tuned to be very accurate methods, and have stability properties that allow for larger time steps than simpler linearization schemes such as fixed-point solvers. The scheme requires a matrix inversion, which is achieved through an application of the Preconditioned Biconjugate Gradient Stabilized (BiCGStab) method, described in Appendix Section B.2. These methods are the foundation for the solver, as well as for the results given in this dissertation, and are reviewed in the Appendix B. In this chapter we describe the approach to the problem in Section 3.2, the prior best effort by Zhang et. al. in Section 3.3, and the method and properties of the Crank-Nicolson based approach in Section 3.4.

Even though great care was taken in [126] to develop an algorithm which captures the spatial derivatives to high accuracy, it turns out that the algorithm is not well suited for long-time integration. In the case of complex or dynamic patterns, an instability caused by the treatment of the non-linear terms in the expression for the temporal derivative causes
the solver to diverge. This is also the case for simulations run over long time periods, such as two thousand frames.

The proposed scheme allows for the simulation of many thousand frames of the Kuramoto-Sivanshinsky (KS) equation, even when the burner radius is made quite large, or noise is added to the system. In the deterministic case, we use the following form of the KS:

\[ \frac{\partial u}{\partial t} = \eta_1 u - (1 + \nabla^2)^2 u - \eta_2 (\nabla u)^2 - \eta_3 u^3. \] (3.1)

The KS (3.1) can be written in polar coordinates as

\[ u_t = -u_{rrrr} - \frac{1}{r^4} u_{\phi\phi\phi} - \frac{2}{r^2} u_{rr\phi\phi} - \frac{2}{r} u_{rrr} + \frac{2}{r^3} u_{r\phi\phi} \]
\[ - \left[ 2 - \frac{1}{r^2} \right] u_{rr} - \left[ \frac{4}{r^4} + \frac{2}{r^2} \right] u_{\phi\phi} - \left[ \frac{1}{r^3} + \frac{2}{r} \right] u_r \] (3.2)
\[ + \eta_1 u - \eta_2 \left[ u_r^2 + \frac{1}{r^2} u_{\phi}^2 \right] - \eta_3 u^3. \]

The equation was augmented through the inclusion of a noise term for the additive noise study as described in Section 5.1, and more specifically in equation 5.1.

### 3.1 The Interpolating Distributed Approximating Functionals

The Interpolating Distributed Approximating Functionals (DAFs) have been extensively described [52, 70, 126, 53, 54, 56] and successfully applied to a wide range of applications, e.g. atom-atom potentials [37], ro-vibrational states of $^3\text{H}_3$ [61], path-integrals for quantal many-body dynamics [69], and the Fokker-Planck equation [127] during the past decade. They are intended for the purpose of approximating a continuous $L^2$ function on a discrete set of points. It is also useful in fitting some linear transformations of the original function, especially in computing the derivatives. We will limit our discussion of DAFs to the Hermite DAF as it is the only form of the DAF used in this thesis.

The DAF is constructed using an approximation to the Dirac $\delta$ function. We formulate our approximation to $f(x)$ and $f^{\ell}(x)$ as follows:

\[ f(x) = \int_{-\infty}^{\infty} \delta(x - x') f(x')dx' \] (3.3)
where the superscript $\ell$ denotes the $\ell$th spatial derivative. The HDAF approximates the Dirac $\delta$ function using the Hermite Polynomials $H_{2n}$ as follows

$$I(x - x') = \frac{1}{\sigma} \exp(-z^2) \sum_{n=0}^{M/2} (-\frac{1}{4})^n \frac{1}{\sqrt{2\pi n!}} H_{2n}(z),$$

(3.5)

where $z = (x - x')/\sigma \sqrt{2}$ while $\sigma$ and $M$ are the DAF parameters. The Gaussian factor $\exp(-z^2)$ dominates the function $I(x - x')$, effectively determining its width. Were we to test the limit of $I$ as $M \to \infty$ or $\sigma \to 0$ we would find that the DAF approaches the Dirac $\delta$ function. Thus using the properties of the Dirac $\delta$ function, the approximation to a function is given by

$$f(x) \approx f_{DAF}(x) = \int_{-\infty}^{\infty} I(x - x') f(x') dx'.$$

(3.6)

The DAF also allows for derivatives of the approximated function to be evaluated as

$$f^{(\ell)}(x) \approx f^{(\ell)}_{DAF}(x) = \int_{-\infty}^{\infty} I^{(\ell)}(x - x') f(x') dx',$$

(3.7)

where $I^{(\ell)}(x - x')$ is defined as the $\ell$th derivative of $I(x - x')$ given by

$$I^{(\ell)}(x - x') = \frac{2^{-\ell/2}}{\sigma^{\ell+1}} \exp(-z^2) \sum_{n=0}^{M/2} (-\frac{1}{4})^n (-1)^{\ell+f} \frac{1}{\sqrt{2\pi n!}} H_{2n+1}(z).$$

(3.8)

Using the known values of grid points the approximation of the DAF is given by

$$f(x) \approx f_{DAF}(x) = \Delta \sum_j I(x - x_j) f(x_j)$$

(3.9)

$$f^{(\ell)}(x) \approx f^{(\ell)}_{DAF}(x) = \Delta \sum_j I^{(\ell)}(x - x_j) f(x_j),$$

(3.10)

where $\Delta$ represents the magnitude of the grid spacing, which we have assumed to be uniform. In our application the quadrature points for the integration are given by the regular grid (FIG. 3.1).

A distinguishing property of the DAFs is the “well tempered” property. A DAF approximation is just as accurate between the grid points as at them. While significant
accuracy can be attained with a small number of basis functions, increased accuracy can be
found by increasing the number of basis functions used. Since the value of the
approximation at any one point is based on a set of surrounding grid points it is flexible
enough for nonlinear systems with complex boundary conditions. Since the approximation is
good at all points of the function we may also state that for any grid spacing \( \Delta \) on the
function there exists a DAF that would give rise to the same approximation, or equally that
from any grid spacing \( \Delta \) one is able to deduce the entire function.

One may make the assumption that by increasing the number of hermitian
polynomials, one is improving the fit of the approximation. This would suggest that an
implementation which used an infinitely high number of hermitian polynomials would, in the
limit, be a perfect fit. However, In studying the application of this method, David Hoffman
et al. [55] discovered that for a fixed grid spacing, the fit improves as the number of
hermitians is increased only up to a point, before beginning to grow worse (likely due to the
propagation of roundoff errors).

3.2 Construction of the Integration Scheme

The problem is solved in polar coordinates because they are the most natural choice
when studying a problem occurring on a circular surface. This choice leads to the problem
of a coordinate singularity that arises from the biharmonic operator,
\[
\nabla^4 = \left( \partial_{rr} + \frac{2}{r} \partial_r + \frac{1}{r^2} \partial_{\phi\phi} \right)^2,
\]
near the origin of the polar grid. Even though the singularity
can be avoided by partitioning each diameter into an even number of equally spaced lattice
points (see FIG. 3.1), the presence of small denominators, \( \frac{1}{r^4} \partial_{\phi\phi\phi\phi} \), at points close to
the origin make the resulting system quite ill-conditioned and extremely sensitive to errors in
the spatial derivatives. Fortunately, the DAFs prove to be accurate enough to approximate
the flame front \( u(r, \phi, t) \) and its spatial derivatives. This is in part due to their broad
support. In fact, near the origin the DAF calculates the radial derivatives, the derivatives
describing the flame front as it crosses the origin, from all of the grid points across the
diameter of the burner.
Figure 3.1. The polar grid. Notice that the innermost points are located at a radius $r = \frac{dr}{2}$, hence there is no computational point at the center of the grid. The radial spacing is $dr$. In our computations we use 32 radial points, and 64 azimuthal points, i.e. $dr = \frac{R}{32}$ and $d\phi = \frac{2\pi}{64}$.

Given the DAF-representation of the spatial derivatives, we now turn our attention to time-integration of the Kuramoto-Sivanshinsky equation. In order to simplify the notation we let $\vec{x} = (r, \phi)$, let $F(\vec{x}, t, u(t))$ represent the right-hand side of the Kuramoto-Sivanshinsky equation (3.1), where for convenience we suppress the dependence on $\vec{x}$. We have

$$u_t(t) = F(\vec{x}, t, u(t)),$$
where \( F(\vec{x}, t, u(t)) \) decomposes into a linear and non-linear operator on \( u(t) \), e.g.
\[
F_{\text{lin}}(\vec{x}, t, u(t)) = -u_{rrrr} - \frac{1}{r^4} u_{\phi\phi\phi\phi} - \frac{2}{r^2} u_{r\phi\phi\phi} - \frac{2}{r} u_{rrr} + \frac{2}{r^3} u_{r\phi\phi} - \left[ \frac{2}{r^2} - 1 \right] u_{rr} - \left[ \frac{4}{r^4} + \frac{2}{r^2} \right] u_{\phi\phi} - \left[ \frac{1}{r^3} + \frac{2}{r} \right] u_r + \eta_1 u
\]
\[
F_{\text{nl}}(\vec{x}, t, u(t)) = -\eta_2 \left[ u_r^2 + \frac{1}{r^2} u_\phi^2 \right] - \eta_3 u^3.
\]

We note that with the DAF-representation every spatial derivative can be expressed as a sum over the domain, with appropriate weights, e.g.
\[
u_{rr}(r, \phi) = \sum_{r_i=1, \phi_i=1}^{N_r, N_\phi} w_{r,DAF}^r (r_i - r, \phi_i - \phi) u(r_i, \phi_i),
\]
where \( \{r_1, r_2, \ldots, r_{N_r}\} \) and \( \{\phi_1, \phi_2, \ldots, \phi_{N_\phi}\} \) represent the discretization of the grid in the radial and azimuthal coordinates, respectively. The weight-coefficients for each derivative only depend on the order of approximation \( M \) and the decay parameter \( \sigma \) in the DAF-description, as well as the grid geometry and can therefore be computed with relative ease. The treatment of the non-linear term \( F_{\text{nl}}(\vec{x}, t, u(t)) \) is more intricate and are the focus of the next 2 Sections 3.3, 3.4.

### 3.3 The Zhang, et. al. Approach

In [126] the proposed DAF-based time-integration scheme for the Kuramoto-Sivanshinsky model is expressed in the form
\[
\frac{u(t+h) - u(t)}{h} = F \left( \vec{x}, t + \frac{h}{2}, \frac{u(t+h) + u(t)}{2} \right),
\]
i.e. the right-hand side is evaluated at the central time \( t + \frac{h}{2} \), in order to achieve second-order accuracy in the time-integration. The non-linear terms, \( F_{\text{nl}}(\vec{x}, t, u(t)) \) give the
following contributions the right-hand-side of (3.13)

\[
\left[\frac{u(t + h) + u(t)}{2}\right]^3 = \frac{1}{8} \left[u(t + h)^3 + 3u(t + h)^2u(t) + 3u(t + h)u(t)^2 + u(t)^3\right]
\]

(3.14)

\[
\left[\frac{u_s(t + h) + u_s(t)}{2}\right]^2 = \frac{1}{4} \left[u_s(t + h)^2 + 2u_s(t + h)u_s(t) + u_s(t)^2\right], \quad s = \{r, \phi\}.
\]

(3.15)

In order to get a linear system in \(u(t + h)\) and its variables, the following linearization is used

\[
\left[\frac{v(t + h) + v(t)}{2}\right]^n \approx \left(1 - \frac{n}{2}\right)v(t)^n + \frac{n}{2}v(t)^{n-1}v(t + h),
\]

yielding

\[
\left[\frac{u(t + h) + u(t)}{2}\right]^3 \approx -\frac{u(t)^3}{2} + \frac{3u(t)^2u(t + h)}{2}
\]

(3.16)

\[
\left[\frac{u_s(t + h) + u_s(t)}{2}\right]^2 \approx u_s(t)u_s(t + h),
\]

(3.17)

where in (3.17) \(s = \{r, \phi\}\). The resulting scheme is unstable for integration over long

periods of time, especially when highly complex patterns are formed. In particular, the errors

in the center of the domain grow exponentially and dominate the solution, generically within

less than a thousand iterations even for relatively simple patterns, one illustration is shown

in FIG. 3.2.

An explanation as to why this exponential error growth should occur follows from

careful analysis of the approximation errors introduced. Taylor expanding equation (3.13)

around \(t + \frac{h}{2}\), shows that the errors due to the non-linear terms on the right-hand side are, to

leading order, of the form

\[
\text{2nd order:} \quad -\eta_2 \left[\frac{1}{4}u_s u_{s tt} - \frac{1}{4}u_{s tt}^2\right] h^2
\]

\[
\text{3rd order:} \quad -\eta_3 \left[\frac{3}{8}u_{tt} u^2 - \frac{3}{4}u_{tt}^2 u\right] h^2.
\]
Figure 3.2. Simulation using the linearization from [126]. The first panel shows the max-norm of the solution, \( \|u(\cdot)\|_{\infty} \), as a function of the number of iterations, it stays relatively constant \( \approx 5 \) for 900 iterations, and then blows up several orders of magnitude with a peak at \( \approx 10^{12} \). The second panel shows a snapshot of the pattern, in which the interior ring rotates clockwise, and the exterior ring rotates counter-clockwise, at iteration 900. The third panel shows the solution at iteration 975, just as the error in the center of the domain starts to dominate the behavior. The fourth panel shows the complete dominance of the error at iteration 1050. The simulation parameters are: \( \eta_1 = 0.32 \), \( \eta_2 = 1 \), \( \eta_3 = 0.017 \), and \( R = 12.0 \).

The second part of the 2nd order error, \( +\eta_2 h^2 u_{xt}^2 / 4 \), is always positive and acts as a de-stabilizing factor. When we compare these errors with the ones introduced in the scheme proposed in the following section (see equations (3.21) and (3.22)), we will notice that the new scheme has a stabilizing factor of the same form. We note that the signs of the remaining three terms that comprise the approximation error are indeterminate and their effects cannot be interpreted as purely stabilizing or de-stabilizing.

3.4 The Crank-Nicolson Based Approach

We now propose a time-integration algorithm that avoids the linearizations in time, see (3.17), used by Zhang et. al. The improved solver allows for simulations to be run for long periods of time. It seems to run just as well for complex and dynamic states as for simple states. It is based on the Crank-Nicolson [23] scheme. With \( F(\vec{x}, t, u(t)) \) as before, we write

\[
\frac{u(t+h) - u(t)}{h} = \frac{F(x, t, u(t)) + F(x, t + h, u(t + h))}{2}. \tag{3.20}
\]

We remark that the Crank-Nicolson scheme is only used for the time-component, the DAF-representation is maintained in order to generate high accuracy approximations to the spatial derivatives. The Crank-Nicolson scheme provides unconditional stability [118]. Taylor expanding (3.20) around \( t + \frac{h}{2} \) shows that the approximation error due to the non-linear
terms are, to leading order

2nd order:
\[-\eta_2 \left[ \frac{1}{4} u_s u_{sst} + \frac{1}{4} u_{st}^2 \right] h^2 \]  \hspace{1cm} (3.21)

3rd order:
\[-\eta_3 \left[ \frac{3}{8} u_{tt} u^2 + \frac{3}{4} u_{t}^2 u \right] h^2. \]  \hspace{1cm} (3.22)

These error terms are very similar to the ones derived for the previous approach, in equations (3.18) and (3.19). The sign of two of the contributing terms have changed, and here the second part of the 2nd order term now provides a stabilizing factor.

We now focus our attention to using the complete non-linear system (3.20) in order to devise a numerical scheme. With the spatial derivatives represented by the DAF-approximations (3.12) we get a non-linear system of equations (3.23)

\[ \vec{G}(\vec{u}(x, t + h)) = 0, \]  \hspace{1cm} (3.23)

where

\[ \vec{G}(\vec{u}(x, t + h)) = \vec{G}_{\text{lin}}(\vec{u}(x, t + h)) + \vec{G}_{\text{nl}}(\vec{u}(x, t + h)), \]  \hspace{1cm} (3.24)

with

\[ \vec{G}_{\text{lin}}(\vec{u}(t + h)) = \left[ \frac{\vec{u}(t + h)}{2} - \frac{\vec{u}(t)}{2} \right] - \left[ \frac{F_{\text{lin}}(x, t + h, \vec{u}(t + h))}{2} + \frac{F_{\text{lin}}(x, t, \vec{u}(t))}{2} \right], \]  \hspace{1cm} (3.25)

\[ \vec{G}_{\text{nl}}(\vec{u}(t + h)) = -\left[ \frac{F_{\text{nl}}(x, t + h, \vec{u}(t + h))}{2} + \frac{F_{\text{nl}}(x, t, \vec{u}(t))}{2} \right], \]  \hspace{1cm} (3.26)

in which \( \vec{u}(\vec{x}, t + h) \) are the unknowns, and \( \vec{u}(\vec{x}, t) \) are known. We solve this using an iterative Newton-based method

\[ \vec{u}^{n+1}(\vec{x}, t + h) = \vec{u}^n(\vec{x}, t + h) - \left[ \delta \vec{G}(\vec{u}^n(\vec{x}, t + h)) \right]^{-1} \cdot \vec{G}(\vec{u}^n(\vec{x}, t + h)), \]  \hspace{1cm} (3.27)

\[ \vec{u}^0(\vec{x}, t + h) = \vec{u}(\vec{x}, t), \]  \hspace{1cm} (3.28)
where \( \delta \vec{G} = \nabla_u \vec{G}(\vec{u}^n(x, t + h)) \) is the Jacobian. The Newton-iteration is repeated until the residual is reduced sufficiently, e.g.,

\[
\| \vec{G}(\vec{u}^{n+1}(x, t + h)) \| \leq \text{tol} \cdot \| \vec{G}(\vec{u}^0(x, t + h)) \|,
\]

in our implementation \( \text{tol} = 10^{-6} \), and the number of required Newton iterations is about 25. In each step of the Newton-iteration we have to solve the linear system

\[
\begin{bmatrix}
\delta \vec{G}(\vec{u}^n(x, t + h))
\end{bmatrix}
\delta \vec{u} = \vec{G}(\vec{u}^n(x, t + h))
\]

in our computational setup, where the grid is subdivided into \( N_r = 32 \) radial points, and \( N_\phi = 64 \) azimuthal points, this leads to a nearly dense \( 2048 \times 2048 \) system. We solve this using the preconditioned bi-conjugate gradient stabilized method (Bi-CGSTAB(\( M \))) [6], where a good preconditioner can be extracted by noticing that the decomposition into linear and non-linear contributions described in equations (3.24), (3.25) and (3.26) of the system is transitive to the Jacobian, and we have

\[
\delta \vec{G}(\vec{u}(x, t + h)) = \delta \vec{G}_{\text{lin}}(\vec{u}(x, t + h)) + \delta \vec{G}_{\text{nl}}(\vec{u}(x, t + h)),
\]

where \( \delta \vec{G}_{\text{lin}}(\vec{u}(x, t + h)) \) is constituted from contributions from DAF-derivative coefficients (3.12) and therefore does not depend on \( \vec{u}(x, t + h) \). We let the linear part define our preconditioner, i.e. \( M = \delta \vec{G}_{\text{lin}}(\vec{u}(x, t + h)) \). The preconditioner \( M \) is used with a fast solver for the linear system \( M \vec{v} = \vec{w} \), based e.g. on the \( LU^- \), or \( QR \)-decomposition of \( M \) which can be computed once for the Bi-CGSTAB(\( M \)) algorithm.
CHAPTER 4
ANALYSIS OF HOPPING STATES IN O(2) SYMMETRIC SYSTEMS

Hopping states represent a specific type of a Modulated Traveling Wave (MTWs). While the cells certainly rotate, this rotation is accompanied by periodic changes in shape and position. The identifying characteristic is the action of an individual cell to make an abrupt change in position, or a hop, while all other cells in its ring continue the group action of rotation. This individual motion is often followed by a hop in the cell immediately following, and likewise continuing around the ring. Hopping behavior was observed as a relatively common sort of dynamic pattern, occurring in single and multiple ring configurations. A review of hopping behavior was published by Gorman et. al. [45] and is summarized in the Appendix Section A.6. Despite their frequent occurrence in physical experimentation they remained suspiciously absent from the prior of simulations of the Kuramoto-Sivanshinsky Equation.

In this chapter the analysis of the three cell hopping cellular pattern (3H) is performed through a decomposition of the high dimensional flame dynamics. The POD discussed in the Appendix Section C.1 is used to generate a lower dimensional model using basis functions that are observed to be similar to the Fourier Bessel functions. With this fact in mind, the Fourier Bessel functions are used in combination as possible lower dimensional basis functions to suggest stability regions, a priori.

While the normal form equations have been described for the k:2k mode interaction [2], they were not known for the hopping state. For this reason we were unable to study the mode interactions underlying the 3H using a normal form analysis prior to our study. However, as a result of our successful simulation we are able to show that in both cases, experiments and computer simulations, hopping states appear to arise from the mutual interaction of three steady-state modes, each mode having Dihedral symmetry. In
Figure 4.1. Four examples of hopping motion, including hopping in the inner ring (13/2H) (a), middle ring (13/5H/1) (b), outer ring (11H/6/1) (c), and outer ring about a single cell (7H/1) (d). This image is reprinted from [45].

In this chapter, we use symmetry-based arguments to derive normal form equations for studying the temporal evolution of the amplitudes associated with these modes. In Section 4.2 we use the Proper Orthogonal Decomposition (POD) and the Fourier-Bessel Decomposition to identify the group of symmetries of the underlying spatial modes that capture the spatial dynamics of hopping states. In Section 4.3 we use the symmetries of the spatial modes to derive a systems of differential equations, in Birkhoff normal form, which governs the temporal evolution of the modes and of the hopping patterns as well. We then perform a bifurcation analysis that promotes understanding, in great detail, of the underlying mechanism that controls the formation and evolution of hopping states. In
Section 4.6 we study the normal form equations to explain the type of bifurcations that lead to hopping states.

4.1 Simulation of the 3 Cell Hopping State

To guide us in the search for specific cellular flame states, we perform a linear stability analysis as follows. First, we assume \( u_0 = 0 \) to be the uniform state or homogeneous flame front that is commonly observed in the experiments. Then we investigate the stability of this uniform state to small perturbations of the form:

\[
w(r, \theta, t) = e^{\lambda t} \Psi_{nm}(r, \theta) + c.c., \quad (4.1)
\]

where \( \Psi_{nm}(r, \theta) = J_n(\alpha_{nm} r / R) e^{im \theta}, \) \((m \geq 0 \) and \( n > 0 \)) and \( J_n(r) \) is the \( n^{th} \) order Bessel function of the first kind and \( \alpha_{nm} \) is its \( m^{th} \) nontrivial zero. It follows that the uniform flame front is stable if \( \lambda < 0 \), and unstable if \( \lambda > 0 \). In physical space, \( \Psi_{nm}(r, \theta) \) has the appearance of a cellular pattern with \( n \) cells whose orientation is determined by \( m \). Thus a perturbation based on Fourier-Bessel functions, some of which are shown in FIG. 4.2, is a natural choice. Now substituting (4.1) into (3.1) and using the fact that

\[
\nabla^2 \Psi_{nm} + k^2 \Psi_{nm} = 0, \quad \text{and} \quad \nabla^4 \Psi_{nm} - k^4 \Psi_{nm} = 0, \quad \text{where} \quad k^2 = (\alpha_{nm} / R)^2,
\]

we arrive at

\[
(\varepsilon - 1 + 2k^2 - k^4 - \lambda)w = 0.
\]

Since we are looking for nontrivial solutions for \( w \), then \( \lambda \) is determined by the roots of characteristic polynomial \( \varepsilon - 1 + 2k^2 - k^4 - \lambda = 0 \). Hence a marginal stability curve, which corresponds to those parameters where \( \lambda = 0 \), is given (as a function of the radius of the burner) by

\[
\varepsilon_{nm}(R) = 1 - 2 \left( \frac{\alpha_{nm}}{R} \right)^2 + \left( \frac{\alpha_{nm}}{R} \right)^4. \quad (4.2)
\]

A critical observation is the fact that beyond this curve, on increasing \( \varepsilon \), the uniform state \( u_0 = 0 \) destabilizes to \( \Psi_{nm}(r, \theta) \). More importantly, we now have a tool to systematically search for the right type of pattern, at least with the right number of cells. Similar marginal stability curves were derived to aid the numerical explorations of cellular patterns in a phenomenological model [92].
Figure 4.2. Fourier Bessel modes used as perturbations in the Stability Analysis. From left to right; the modes in the first row are $\Psi_{11}$, $\Psi_{12}$, $\Psi_{13}$, the modes in the second row are $\Psi_{21}$, $\Psi_{22}$, $\Psi_{23}$, the modes in the third row are $\Psi_{31}$, $\Psi_{32}$, and $\Psi_{33}$.

The 3H state was known from physical experiments to be composed of three different stable modes, including the $\Psi_{21}$, $\Psi_{31}$, $\Psi_{41}$. The stability analysis provides a region to which the evolution of a single-ring pattern with three cells can be traced. Such a region can be found in a neighborhood of the minimum of the marginal stability curve $B_{31}$ shown in FIG. 4.3. As the curved is crossed, on increasing $R$, a stationary pattern of three cells with purely spatial $D_3$ symmetry emerges via a symmetry-breaking bifurcation from the O(2)-invariant trivial solution.
Figure 4.3. Marginal stability curves outline the stability domains where the trivial solution \( u_0 = 0 \) (representing a uniform flame front) bifurcates to Fourier-Bessel modes \( \Psi_{nm} \). The shaded region displays the parameter region in which the 3H state was found in simulations.

Increasing \( R \) further, and upon crossing the left edge of the shaded region, the three-cells pattern loses stability, the \( D_3 \) symmetry of the ring is broken, and a dynamic pattern of three cells rotating rigidly and counter-clockwise bifurcates subcritically. FIG. 4.4 depicts various snapshots of the evolution of the \( u(r, \theta, t) \) field obtained at \( R = 7.36 \). Observe that the shape of the cells remains, approximately, constant as the ring rotates.

Figure 4.4. Ten sequential time (top index) snapshots of a dynamic state of three cells rotating counter-clockwise, with small modulations, found in simulations of (3.1). Parameter values are: \( \eta_1 = 0.32, \eta_2 = 1.0, \eta_3 = 0.013, \) and \( R = 7.36 \).
An ensemble of 2000 consecutive snapshots was generated for the POD analysis. FIG. 4.5 shows the time-average (can be considered mode $\Phi_0$) followed by the ten modes, $\Phi_1 - \Phi_{10}$, with the highest POD energy (see C.1 for an exact definition). The actual amount of energy in each mode is indicated below each graph. Each mode shows some amount of symmetry. The symmetry of the time-average, in particular, reflects the $O(2)$-symmetry of the burner, even though none of the instantaneous snapshots has this symmetry. This feature is studied in more detail in [29]. The remaining ten modes exhibit, approximately, the following symmetries: $\Phi_1$ and $\Phi_2$ have $D_3$-symmetry, meaning that one third of a revolution leaves them unchanged; $\Phi_3$ and $\Phi_4$ show $D_1$-symmetry, i.e., the patterns are restored after one complete revolution; $\Phi_5$ and $\Phi_6$ exhibit $D_6$-symmetry, which is just a higher harmonic of the first two modes $\Phi_1$ and $\Phi_2$; $\Phi_7$ and $\Phi_8$ are $D_2$-symmetric; and $\Phi_9$ and $\Phi_{10}$ are $D_4$-symmetric. Observe also that the energy is almost equally distributed between consecutive pairs of modes, indicating the existence of coupling pairs or invariant subspaces for reconstructing the dynamics: $V_3 = \text{span}\{\Phi_1, \Phi_2\}$, $V_1 = \text{span}\{\Phi_3, \Phi_4\}$, $V_6 = \text{span}\{\Phi_5, \Phi_6\}$, $V_2 = \text{span}\{\Phi_7, \Phi_8\}$, and $V_4 = \text{span}\{\Phi_9, \Phi_{10}\}$, where the index $n$ in $V_n$ indicates $D_n$-symmetry.

![Figure 4.5](image)

**Figure 4.5.** POD decomposition of a single ring state with three cells rotating uniformly and counter-clockwise.
The fact that five pairs of modes are needed to capture about 95% of the energy is in clear contrast to the energy distribution of certain uniformly rotating cells that were studied through simulations of a phenomenological model and simulations of the KS model as well [94, 93]. Such uniformly rotating cells were also created via steady-state mode interaction but only two pairs of modes were needed to capture almost 100% of the energy. Another significant difference is the fact the Dihedral group of symmetries of the invariant subspaces found in the decomposition of the uniformly rotating cells are in a 1:2 ratio. These assertions suggest that the cells of the state shown in FIG. 4.4 do not rotate uniformly and that they are created via a steady-state mode interaction through the spaces \( V_3 \oplus V_1 \oplus V_6 \oplus V_2 \oplus V_4 \). Phase-space projections and relative phase angles shown in FIG. 4.6 further confirm that the pattern rotates non-uniformly. The temporal modulations are visible in the graph of \( a_7 \) vs \( a_8 \) and in the associated relative phase angles that appears just below it. Clearly the modulations are very small but this is the case because the pattern is very close to its bifurcation point, i.e., it appears just slightly to the right of \( R = 7.36 \). Recall that to the left of \( R = 7.36 \) the three cell state becomes stationary.

Computer animations of the reconstructed dynamics through

\[
\begin{align*}
    u(x, t) = \tilde{u} + \sum_{k=1}^{M} a_k(t) \Phi_k(x)
\end{align*}
\]  

(4.3)

show the following features. With \( M = 2 \) modes, a dynamic state emerges with three cells rotating counter-clockwise and almost rigidly (under the naked eye). The asymmetry on each individual cell is almost indistinguishable, but we know from previous work [48, 94] that rotating cells can not posses reflectional (also called “chiral”) symmetry. The argument is straightforward. If a solution (cellular state) of a system of differential equations has certain symmetries at one instant of time, then that solution must have the same symmetries at all times. Consequently, any cellular state with reflectional symmetry cannot rotate. With \( M = 4 \) modes, however, the asymmetry in the cells becomes more visible. The cells do not seem to change shape too much, but rather, it is their size that periodically increases and then decreases as the cells rotate. With \( M = 6 \), the cells behave in a similar
Figure 4.6. (left) Phase-space projections and (b) phase-angles produced by the time coefficients of the POD decomposition of the rotating pattern shown in FIG. 4.4 suggest that the pattern rotates uniformly.

manner except that their size increases moderately. With $M = 8$, the asymmetry in the cells is more pronounced as well as the variations in shape. Also the cells move more independently with small “jumps” in angular position. With $M = 10$, the jumps are more visible and the overall temporal motion shows similar characteristics to those of experimental hopping states [45, 92]. This last assertion is not a big surprise given the fact that in a POD decomposition of experimental hopping states similar modes to those shown in FIG. A.8 were found. In particular, the $\Phi_1$, $\Phi_2$, $\Phi_7$, $\Phi_8$, $\Phi_9$, and $\Phi_{10}$ modes were found to be the most dominant modes. It is a surprise, however, that $\Phi_3 - \Phi_6$ do not appear in the experimental states, not even at lower energy levels. To understand this subtle difference, we performed a numerical experiment of reconstructing the dynamics without $\Phi_3, \Phi_4$, and
Interestingly, the reduced reconstructed dynamics resemble more of the hopping motion that is typically observed in the experiments. This better-fit can be attributed to the fact that now the spatial dynamics are stripped from the oscillations in cell size (without changing shape) that we previously observed in the reconstructions with $M = 4$ and $M = 6$. Consequently, the periodic “hops” in angular position are more distinguishable.

We now return our attention to the marginal stability curves. On moving right into the shaded region, the modulations on the three-cells state of FIG. 4.4 become progressively stronger. Near $R = 7.74$, in particular, the cells repeatedly make abrupt changes in their angular position while they rotate around the ring; in a manner that closer resembles experimental observations of hopping cells [43, 45]. FIG. 4.7 depicts a few representative snapshots of the spatio-temporal dynamics at $R = 7.7475$. Observe that changes in cell shape are more noticeable. In fact, a hopping cell changes its shape more than the other two and also appears more asymmetric. The hops are small in comparison with experimental states but, up to a time-scale factor, the overall characteristics of the dynamics appear to be in good agreement with experiments. To confirm these observations, we perform next a POD analysis of the space-time behavior.

![Figure 4.7. Space and time evolution of a three-cell hopping state found in simulations of (3.1). The cells move nonuniformly and their shapes change periodically. Parameter values are: $\eta_1 = 0.32$, $\eta_2 = 1.0$, $\eta_3 = 0.013$, and $R = 7.7475$.](image-url)
An ensemble of 6000 consecutive snapshots was generated for the POD decomposition. FIG. 4.8 shows the time-average, principal modes, and POD energy, in the same format as they appeared in FIG. 4.5. A direct comparison of the modes yields the following observations. The invariant subspaces $V_3, V_2$, and $V_4$ are present in both cases. Modes $\Phi_3, \Phi_4$, and $\Phi_5$, in FIG. 4.8, do not appear in FIG. 4.5. Mode $\Phi_{10}$ in FIG. 4.8 corresponds to mode $\Phi_{11}$ in FIG. 4.5, though this mode is not shown in FIG. 4.5. Modes $\Phi_3$ and $\Phi_4$ in FIG. 4.8 can be though of being a linear superposition of two concentric modes with $D_1$-symmetry. In this sense, they are similar to the same modes $\Phi_3$ and $\Phi_4$ of FIG. 4.8.

Individually, the dynamics of each cell appears more complicated however. The sequence of snapshots reveals (see frames 0 and 120) small but visible jumps in the angular position of each cell. A jumping cell changes its shape more than the other two and also appears more asymmetric. The jumps are small in comparison with experimental observations of hopping states but, up to a time scale factor, the general characteristics of the dynamics are very similar to that of hopping states.

FIG. 4.8 shows the POD modes extracted from an ensemble made up of 6000 snapshots. Observe that the time average also reflects the $O(2)$ symmetry of the burner. Below the time average, the eight most energetic POD modes $\Phi_1-\Phi_8$ are shown. FIG. 4.9 shows the phase plane plots for the most energetic modes.

Computer animations of the reconstructed dynamics through Equation 4.3 shows the following features. With $M = 2$ modes, a three-cell dynamic pattern emerges, the cells rotate counter-clockwise and their size and shape is relatively constant at all times. With $M = 4$ modes, the cells now periodically change shape, each cell takes turns changing size, increasing as it moves closer to the edge of the simulated burner and decreasing as it moves towards the center of the burner. This behavior supports the interpretation of $\Phi_3$ and $\Phi_4$ as being made up of two concentric modes with $D_1$-symmetry. With $M = 5$ modes, the excursions towards the center and boundary of the burner are more noticeable. The smallest cell is always the one pulled towards the center of the burner, just before the leading cell
makes an abrupt hop towards the preceding cell. This pulling effect occurs everywhere around the center of the burner, which explains the apparent loss of structure in the fifth mode. With $M = 7$ the cells look more asymmetric with larger changes in shape. With $M = 9$ modes, each cell periodically makes abrupt changes of angular position, jumping closer to the cell immediately in front as shown in FIG. 4.10. This type of hopping motion is clearly more noticeable as compared to the small jumps seen in the previous dynamic state of FIG. 4.4.

The thickness in the phase-space projections of the POD time coefficients, see FIG. 4.9, confirms the presence of stronger temporal modulations as compared to those seen in FIG. 4.6. Stronger modulations explain why the hopping behavior is now more noticeable. Computer animations of the numerical results will be posted online at http://terminus.sdsu.edu/ks/.

Hence, except for the periodic excursions between the center and boundary of the burner, the spatio-temporal features described by the dynamic state of FIG. 4.7 are in good agreement with experimental observations of hopping motion [45, 92]. The excursions are governed by modes $\Phi_3$, $\Phi_4$, and $\Phi_5$ of FIG. 4.8. Removing these modes (and $\Phi_{10}$ to make the comparison relevant to the states shown in FIG. A.8) we observe a dynamic state with
Figure 4.9. (Top) Phase-space projections produced by the time coefficients of the POD decomposition of the rotating pattern shown in FIG. 4.7; (bottom) Associated relative phase angles.

Figure 4.10. Reconstruction of the hopping state with $M = 9$ modes.

spatio-temporal characteristics as shown in FIG. 4.11. The result is strongly similar to those seen in FIG. A.8, especially in column (a).
4.2 Symmetry Identification and Steady-State Modes

FIG. 4.12 shows the results of a Proper Orthogonal Decomposition decomposition of the two three-cell hopping states of FIG. A.8, i.e. one state where three cells hop in a single ring and one where the cells hop within a steady outer ring. In the former case, cells are numbered for identification purposes. In frame 1, cell 1 is just finishing a hop. The cell behind it, cell 3, then begins to move in frame 2 and completes its hop in frame 3. It is then the turn for cell 2 to hop and its motion is completed in frame 4. In frame 5, the cycle repeats over again starting with cell 1. Observe that cells appear more asymmetric and move faster when they are hopping. In both cases, the time average of the images $\bar{u}$ are shown in the middle-top snapshot followed below by the six most energetic POD modes, ordered from left-to-right and top-to-bottom. An approximation with these six modes is shown in column (c) of each individual state. Since the POD modes were obtained directly from video images of the combustion experiments, their analytical form are unknown. However, their symmetries can be estimated through the Fourier-Bessel decomposition

$$u(r, \theta, t) = \sum_{n,m} z_{nm}(t) \Psi_{nm}(r, \theta) + c.c.$$  \hspace{1cm} (4.4)$$

where $\Psi_{nm}(r, \theta) = J_n(\alpha_{nm} r / R) e^{im\theta}$, $(m \geq 0$ and $n > 0)$ and c.c. denotes complex conjugate [123]. Here $J_n(r)$ is the $n^{th}$ order Bessel function of the first kind and $\alpha_{nm}$ is its
The \( m^{th} \) nontrivial zero, \( z_{nm} \), are complex time-dependent coefficients, save for \( z_{0m} \), which are real. For the first three pairs, we find the largest contributions to come from Fourier-Bessel modes \( \Psi_{21}, \Psi_{31}, \) and \( \Psi_{41} \), respectively. This confirms our visual perception that the underlying symmetries of each consecutive pair of modes are described, approximately, by the Dihedral groups \( D_2, D_3, \) and \( D_4 \) respectively, where \( D_n \) is the group of symmetries—rotations and reflections—of an \( n \)-gon.

![Figure 4.12. POD decomposition of hopping motion in (left) a single three-cell ring; and in (right) an inner ring of three cells surrounded by a stationary outer ring with eleven cells. In both cases: (a) five instantaneous snapshots depicting hopping motion; (b) time-average of the data set appears at the top, followed (from left-to-right and top-to-bottom) by the six most energetic steady-state POD modes; and (c) reconstruction of the dynamics using the six most energetic POD modes.](image-url)

We now turn our attention to the numerical hopping state depicted in FIG. 4.7. The results of the POD analysis are shown in FIG. 4.13, which depicts the time-average (considered mode \( \Phi_0 \)) followed by the ten modes, \( \Phi_1-\Phi_{10} \), with the highest POD energy. The actual amount of energy in each mode is indicated below each graph. Each mode shows some amount of symmetry. Observe that except for modes \( \Phi_3, \Phi_4, \) and \( \Phi_5 \), all other modes
(including the time-average) do appear in the POD analysis of the experimental hopping states, see FIG. 4.12. \( \Phi_{10} \) also appears in FIG. 4.12 but it is not shown since it contains very little energy. Carefully examination of the POD-reconstructed dynamics through

\[
u(x, t) = \bar{u} + \sum_{k=1}^{M} a_k(t) \Phi_k(x),
\]

where \( \bar{u} \) is the time-average of the data set \( u(x, t) \), reveals a subtle difference between the POD-reconstructed dynamics and the actual experiments. Modes \( \Phi_3, \Phi_4, \) and \( \Phi_5 \), lead the cells to make periodic excursions between the boundary and the center of the circular domain, all while they hop around the ring. This feature is only observed in computer simulations of the KS model and not in experiments. It can be attributed to the lack of external noise and/or fluctuations in burner temperature. However, computer animations of the reconstructed dynamics, excluding modes \( \Phi_3, \Phi_4, \) and \( \Phi_5 \), show a dynamic state whose spatio-temporal characteristics are in very good agreement with those of experiments. Hence, up to these subtle differences, it is reasonable to identify the Fourier-Bessel modes \( \Psi_{21}, \Psi_{31}, \) and \( \Psi_{41} \), as the principal modes of hopping states, including experiments and numerics. Thus we can write:

\[
u(x, t) = \bar{u} + z_2(t)\Psi_{21}(x) + z_3(t)\Psi_{31}(x) + z_4(t)\Psi_{41}(x) + c.c.
\]

Next we exploit the \( \text{O}(2) \)-symmetry of the burner to derive normal form equations for the time-amplitude coefficients \( z_2, z_3, \) and \( z_4 \).

### 4.3 Equivariant Normal Forms

We now consider an idealization of the flame experiment by a \( \Gamma \)-equivariant system of ODEs

\[
\frac{dz}{dt} = f(z, \mu),
\]

where \( \Gamma = \text{O}(2) \) represents the circular symmetry of the burner, \( z = (z_2, z_3, z_4) \in \mathbb{C}^3 \), and \( \mu \in \mathbb{R}^3 \) are vectors of parameters. We assume \( z = 0 \) to be the \( \text{O}(2) \)-symmetric “trivial solution” (planar front) of the experiment satisfying

\[
f(0, \mu) = 0.
\]
We also assume that \( f \) has a steady-state bifurcation at \( \mu = (0, 0, 0) \), so that \( V = \ker(Df) \) is nonzero. In particular, for a three steady-state mode interaction we consider the linear degeneracy where the linearization \( L = (Df)_{0,(0,0,0)} \) has three zero eigenvalues. Thus we assume

\[
V = V_2 \oplus V_3 \oplus V_4,
\]

where \( V_k = \text{span}\{Re\{\Psi_{k1}\}, Im\{\Psi_{k1}\}\}, k = 2, 3, 4 \). Under these assumptions, at \( \mu = (0, 0, 0) \), the \( z = 0 \) uniform solution loses stability and three \( \text{O}(2) \) symmetry–breaking branches of steady-states modes interact with each other. The action of \( \Gamma \) on \( C^3 \) is generated by

\[
\begin{align*}
\theta \cdot (z_2, z_3, z_4) &= (e^{2\theta i}z_2, e^{3\theta i}z_3, e^{4\theta i}z_4), \quad (\theta \in \text{SO}(2)), \\
\kappa \cdot (z_2, z_3, z_4) &= (\bar{z}_2, \bar{z}_3, \bar{z}_4), \quad (\kappa = \text{flip}).
\end{align*}
\]

### 4.4 O(2)-Invariants and O(2)-Equivariants

**Proposition 4.1** Every real-valued \( \text{O}(2) \)-invariant germ is a function of \( \rho_k \) and \( v_k \), \( k = 2, 3, 4 \), where

\[
\begin{align*}
\rho_2 &= |z_2|^2, & \rho_3 &= |z_3|^2, & \rho_4 &= |z_4|^2, \\
v_2 &= z_3^2\bar{z}_1 + \bar{z}_3z_1^2, & v_3 &= z_2^2\bar{z}_4 + \bar{z}_2z_4^2, & v_4 &= z_2^2\bar{z}_3 + \bar{z}_2z_3^2.
\end{align*}
\]
**Proof:** The general $O(2)$-invariants can be written as

$$f(z) = \sum a_{a_2a_3a_4} z_2^a z_3^b z_4^c.$$ 

SO(2) invariance of $f$, i.e. $f(\theta z) = f(z)$ implies that $a_{a_2a_3a_4} = 0$, unless

$$2(\alpha_2 - \beta_2) + 3(\alpha_3 - \beta_3) + 4(\alpha_4 - \beta_4) = 0. \quad (4.9)$$

We may assume $(\alpha_2 - \beta_2) = 0$ or $(\alpha_3 - \beta_3) = 0$ or $(\alpha_4 - \beta_4) = 0$ or $(\alpha_2 - \beta_2) = 3 \times 4 \times s$, $(\alpha_3 - \beta_3) = 2 \times 4 \times s$, $(\alpha_4 - \beta_4) = -2 \times 3 \times s$, for some positive integer $s$. If $(\alpha_2 - \beta_2) = 0$, for instance, then

$$\alpha_3 - \beta_3 = 4k,$$

$$\alpha_4 - \beta_4 = -3k,$$

for some positive integer $k$. We can then write

$$f(z) = \sum a_{a_2a_3a_4} (z_2 z_3)'' a_2 (z_3 z_4)'' a_3 (z_4 z_4)'' a_4 (z_4 z_4)'' k.$$ 

This case, i.e. $(\alpha_2 - \beta_2) = 0$, leads to generators $\rho_2 = |z_2|^2$, $\rho_3 = |z_3|^2$, $\rho_4 = |z_4|^2$, and $z_3^4 z_4^3$. Similarly, $(\alpha_3 - \beta_3) = 0$ leads to generators $\rho_2$, $\rho_3$, $\rho_4$, and $z_2^3 z_4$.

The last case where $(\alpha_4 - \beta_4) = 0$, yields generators $\rho_2$, $\rho_3$, $\rho_4$, and $z_2^3 z_2$. The last case where $(\alpha_2 - \beta_2) = 3 \times 4 \times s$, etc., does not yield any new generators. Finally invariance under $\kappa$, i.e. $f(\kappa z) = f(z)$, leads to the final set of generators $z_3^4 z_4^3 + z_3^4 z_4^3$, $z_2^3 z_4 + z_2^3 z_4$, and $z_2^3 z_2 + z_2^3 z_2$. 

**Proposition 4.2** The $O(2)$-equivariant germs $f : \mathbb{C}^3 \rightarrow \mathbb{C}^3$ are generated over the $O(2)$-invariants by the following mappings:

- $V^1 = (z_2, 0, 0)$,
- $V^2 = (0, z_3, 0)$,
- $V^3 = (0, 0, z_4)$,
- $V^4 = (z_2, z_3, 0)$,
- $V^5 = (0, z_2, 0)$,
- $V^6 = (z_2, z_4, 0, 0)$,
- $V^7 = (0, z_2, z_4, 0)$,
- $V^8 = (0, 0, z_2, z_4)$,
- $V^9 = (z_2, z_3, 0, 0)$,
- $V^{10} = (z_2, z_4, 0, 0)$,
- $V^{11} = (0, 0, z_3, 0)$,
- $V^{12} = (0, z_3, z_4, 0, 0)$,
- $V^{13} = (0, 0, z_3, z_4)$. 

Proof: Let \( f(z) = (f_2, f_3, f_4) \) be an \( O(2) \)-equivariant mapping \( f: \mathbb{C}^3 \rightarrow \mathbb{C}^3 \). Write \( f_2 \) as follows

\[
f_2(z) = \sum a_{\alpha_2 \beta_2 \alpha_3 \beta_3 \alpha_4 \beta_4} z_2^\alpha \bar{z}_2^\beta z_3^\alpha \bar{z}_3^\beta z_4^\alpha \bar{z}_4^\beta.
\]

Commutativity of \( f \) with \( SO(2) \) implies that \( e^{2\theta_i} f_2(z) = f_2(e^{2\theta_i} z_2, e^{3\theta_i} z_3, e^{4\theta_i} z_4) \), so that \( a_{\alpha_2 \beta_2 \alpha_3 \beta_3 \alpha_4 \beta_4} = 0 \) unless

\[
2(\alpha_2 - \beta_2 - 1) + 3(\alpha_3 - \beta_3) + 4(\alpha_4 - \beta_4) = 0.
\]

An analysis similar to that of Eq. (4.9) yields, modulo the \( O(2) \)-invariants, generators \( V^1, V^4, V^6, V^9, \) and \( V^{10} \).

Next we write \( f_3 \) as follows

\[
f_3(z) = \sum a_{\alpha_2 \beta_2 \alpha_3 \beta_3 \alpha_4 \beta_4} z_2^\alpha \bar{z}_2^\beta z_3^\alpha \bar{z}_3^\beta z_4^\alpha \bar{z}_4^\beta.
\]

Commutativity of \( f \) with \( SO(2) \) implies that \( e^{3\theta_i} f_3(z) = f_3(e^{2\theta_i} z_2, e^{3\theta_i} z_3, e^{4\theta_i} z_4) \), so that \( a_{\alpha_2 \beta_2 \alpha_3 \beta_3 \alpha_4 \beta_4} = 0 \) unless

\[
2(\alpha_2 - \beta_2) + 3(\alpha_3 - \beta_3 + 1) + 4(\alpha_4 - \beta_4) = 0.
\]

An analysis similar to that of Eq. (4.9) yields, modulo the \( O(2) \)-invariants, generators \( V^2, V^7, V^{11}, \) and \( V^{12} \).

Finally we write \( f_4 \) as follows

\[
f_4(z) = \sum a_{\alpha_2 \beta_2 \alpha_3 \beta_3 \alpha_4 \beta_4} z_2^\alpha \bar{z}_2^\beta z_3^\alpha \bar{z}_3^\beta z_4^\alpha \bar{z}_4^\beta.
\]

Commutativity of \( f \) with \( SO(2) \) implies that \( e^{4\theta_i} f_4(z) = f_4(e^{2\theta_i} z_2, e^{3\theta_i} z_3, e^{4\theta_i} z_4) \), so that \( a_{\alpha_2 \beta_2 \alpha_3 \beta_3 \alpha_4 \beta_4} = 0 \) unless

\[
2(\alpha_2 - \beta_2) + 3(\alpha_3 - \beta_3) + 4(\alpha_4 - \beta_4 - 1) = 0.
\]

An analysis similar to that of Eq. (4.9) yields, modulo the \( O(2) \)-invariants, generators \( V^3, V^5, V^8, \) and \( V^{13} \).
4.5 Branching Equations

It follows from Propositions 4.1 and 4.2 that the general $\mathbf{O}(2)$-equivariant mapping

$$f(z, \mu_2, \mu_3, \mu_4) \in \mathbb{C} \times \mathbb{C}^3$$

has the form

$$f = A_1 \begin{bmatrix} z_2 \\ 0 \end{bmatrix} + A_2 \begin{bmatrix} 0 \\ 0 \end{bmatrix} + A_3 \begin{bmatrix} z_3^2 \bar{z}_4 \\ 0 \end{bmatrix} + A_4 \begin{bmatrix} 0 \\ 0 \end{bmatrix} + A_5 \begin{bmatrix} 0 \\ 0 \end{bmatrix} + B_1 \begin{bmatrix} 0 \\ z_3 \end{bmatrix} + B_2 \begin{bmatrix} 0 \\ z_2 \bar{z}_3 \end{bmatrix} + B_3 \begin{bmatrix} 0 \\ z_3^2 \bar{z}_4 \end{bmatrix} + B_4 \begin{bmatrix} 0 \\ z_2 \bar{z}_3 \end{bmatrix}$$

$$+ C_1 \begin{bmatrix} 0 \\ z_4 \end{bmatrix} + C_2 \begin{bmatrix} 0 \\ z_2^2 \end{bmatrix} + C_3 \begin{bmatrix} 0 \\ z_2 z_3^2 \end{bmatrix} + C_4 \begin{bmatrix} 0 \\ z_3^2 \bar{z}_4 \end{bmatrix},$$

(4.10)

where $A_i$, $B_i$, and $C_i$ are complex-valued $\mathbf{O}(2)$-invariant functions depending on three parameters $\mu_2$, $\mu_3$, and $\mu_4$. Additionally, the eigenvalue structure of $f$ leads to $A_1(0) = 0$, $B_1(0) = 0$, and $C_1(0) = 0$.

Computer simulations of the KS model (3.2) reveal that if we decrease the primary bifurcation parameter (radius of the burner), near a hopping state, then the abrupt changes of angular positions that characterize hopping states, see FIG. 4.7, become less visible. A dynamic pattern would exhibit (under the naked eye) more characteristics of a traveling wave state, i.e. the cells rotate almost uniformly and almost rigidly with little change in shape. This critical observation leads us to believe that hopping states in the KS model are modulated traveling waves that emerge from the bifurcation of traveling wave solutions. To explore further this assertion, we consider next the stability properties of traveling wave solutions of (4.10), which emerge from the interaction of the three steady-state modes $\Psi_{21}$, $\Psi_{31}$, and $\Psi_{41}$. Using (4.10), we re-scale and re-write the general $\mathbf{O}(2)$-equivariant, up to
third order, as follows

\[\begin{align*}
\dot{z}_2 &= \bar{z}_2 z_4 + \alpha_2 z_2^2 \bar{z}_4 + z_2 (\mu_2 + e_{22} |z_2|^2 + e_{24} |z_4|^2) \\
\dot{z}_3 &= \alpha_3 z_2 \bar{z}_3 z_4 + z_3 (\mu_3 + e_{32} |z_2|^2 + e_{34} |z_4|^2) \\
\dot{z}_4 &= \pm z_2^2 + \alpha_4 z_2^3 \bar{z}_2 + z_4 (\mu_4 + e_{42} |z_2|^2 + e_{44} |z_4|^2),
\end{align*}\]

(4.11)

where \(\alpha_2, \alpha_3,\) and \(\alpha_4,\) are real-valued constants.

### 4.6 Bifurcation Analysis

We observe that the governing equations (4.11) are similar to those considered by Campbell and Holmes [25] in the study of heteroclinic cycles that result from the interaction of three complex Fourier modes whose wave numbers are in a \(k : 2k : 4k\) ratio, except that now mode \(\Psi_{31}\) replaces mode \(\Psi_{11}\) and the ratio is no longer valid. We also observe that the four-dimensional subspace \(z_3 = 0\) is invariant under (4.11), leading to a \(k : 2k\) mode interaction analogous to the \(1 : 2\) mode interaction studied by Armbruster [2]. Consequently, we will draw extensively on the methods and results of Campbell et al. and on those of Armbruster et al.

#### 4.6.1 Mixed Modes and Traveling Wave Solutions

Guided by the critical observation that near the onset of hopping states the overall dynamic pattern resembles a traveling wave, we study in this section the stability properties of traveling wave solutions of (4.11). These solutions are known to bifurcate from a mixed mode \((z_2 \neq 0, z_4 \neq 0)\) solution in the invariant space \(z_3 = 0\), given by

\[\begin{align*}
\dot{z}_2 &= \bar{z}_2 z_4 + z_2 (\mu_2 + e_{22} |z_2|^2 + e_{24} |z_4|^2) \\
\dot{z}_4 &= \pm z_2^2 + z_4 (\mu_4 + e_{42} |z_2|^2 + e_{44} |z_4|^2).
\end{align*}\]

(4.12)

For convenience, we let \(z_j = re^{\phi_j}\) and \(\phi_2 = 2\theta_2 - \theta_4\), so that we can rewrite (4.12) in polar coordinates

\[\begin{align*}
\dot{r}_2 &= r_2 r_4 \cos \phi_2 + r_2 (\mu_2 + e_{22} r_2^2 + e_{24} r_4^2) \\
\dot{r}_4 &= \pm r_2^2 \cos \phi_2 + r_4 (\mu_4 + e_{42} r_2^2 + e_{44} r_4^2) \\
\dot{\phi}_2 &= -\left(\frac{2r_4 \pm r_2^2}{r_4}\right) \sin \phi_2.
\end{align*}\]

(4.13)
We are interested in the $\pi$-mixed mode solution of Armbruster et al., in which $\phi_2 = \pi$, while $r_2 \neq 0$ and $r_4 \neq 0$ are given by the simultaneous solution of

\[
\begin{align*}
-r_2 r_4 &+ r_2 (\mu_2 + e_22 r_2^2 + e_24 r_4^2) = 0 \\
r_2^2 &+ r_4 (\mu_4 + e_42 r_2^2 + e_44 r_4^2) = 0.
\end{align*}
\] (4.14)

Following Armbruster et al., traveling waves are equilibria of (4.13) with $\phi_2 \neq 0, \pi$. They are created via a pitchfork bifurcation, in the $\phi_2$ direction, from the $\pi$-mixed modes when $2r_4 \pm r_2^2/4 = 0$ and $\phi_2 = \pi$, so that they only exist in the "-" case or when $r_2^2 = 2r_4^2$. Letting $r_4 = \rho$ and $e = 4e_22 + 2e_24 + 2e_42 + e_44$, we get

\[
\begin{align*}
\rho^2 &= -\frac{(2\mu_2 + \mu_4)}{e} \\
\cos \phi_2 &= \frac{\mu_4 (2e_22 + e_44) - \mu_2 (2e_42 + e_44)}{-\sqrt{(2\mu_2 + \mu_4)e}}.
\end{align*}
\] (4.15)

Since traveling waves emerge at $\phi_2 = \pi$, we also get, in $(\mu_2, \mu_4)$-space, the following bifurcation set

\[
\mu_4 = -2\mu_2 - e\mu_2^2 + O(\mu_2^3).
\] (4.16)

Furthermore, within the $(z_2, z_4)$ subspace, traveling waves exist and are stable for

\[
-2\mu_2 - e\mu_2^2 + O(\mu_2^3) < \mu_4 < \mu_2 \left(1 + \frac{9(e_{44} - e_{24})}{e - 3(e_{44} - e_{24})}\right) + O(\mu_2^3).
\] (4.17)

Next we consider the stability of the traveling wave solutions in the $z_3$-direction. Again, for convenience we let $z_j = r e^{\theta_j}$, $\phi_2 = 2\theta_2 - \theta_4$, $\phi_3 = 2\theta_3 - (\theta_2 + \theta_4)$, and re-write the full system (4.11) in polar coordinates as follows

\[
\begin{align*}
\dot{r}_2 &= r_2 r_4 \cos \phi_2 + \alpha_2 r_3^2 r_4 \cos \phi_3 + r_2 (\mu_2 + e_22 r_2^2 + e_23 r_3^2 + e_24 r_4^2) \\
\dot{r}_3 &= \alpha_3 r_2 r_3 r_4 \cos \phi_3 + r_3 (\mu_3 + e_32 r_2^2 + e_33 r_3^2 + e_34 r_4^2) \\
\dot{r}_4 &= \pm r_4^2 \cos \phi_2 + \alpha_4 r_2^2 r_4 \cos \phi_3 + r_4 (\mu_4 + e_42 r_2^2 + e_43 r_3^2 + e_44 r_4^2) \\
\dot{\phi}_2 &= -\left(2r_4 \pm \frac{r_2^2}{r_4}\right) \sin \phi_2 + \left(2\alpha_2 r_3^2 r_4 \frac{r_2}{r_2} - \alpha_4 r_2 r_3 \frac{r_3}{r_4}\right) \sin \phi_3 \\
\dot{\phi}_3 &= \left(r_4 \mp \frac{r_2^2}{r_4}\right) \sin \phi_2 - \left(2\alpha_3 r_2 r_4 + \alpha_2 r_3^2 r_4 \frac{r_2}{r_2} + \alpha_4 r_2 r_3 \frac{r_3}{r_4}\right) \sin \phi_3,
\end{align*}
\] (4.18)
where
\[\begin{align*}
\dot{\theta}_2 &= -r_4 \sin \phi_2 + \alpha_2 \frac{r_3^2 r_4}{r_2} \sin \phi_3 \\
\dot{\theta}_3 &= \alpha_3 r_2 r_4 \sin \phi_3 \\
\dot{\theta}_4 &= \pm \frac{r_2^2}{r_4} \sin \phi_2 + \alpha_4 \frac{r_2 r_3^2}{r_4} \sin \phi_3.
\end{align*}\] (4.19)

In order to avoid the coordinate singularity at \( r_3 = 0 \), we use the following mixed Cartesian/polar representation of mode \( z_3 = x_3 + y_3 i \).

\[
\begin{bmatrix}
\dot{x}_3 \\
\dot{y}_3
\end{bmatrix} =
\begin{bmatrix}
\alpha_3 r_2 r_4 \cos \theta_{24} + \mu_3 + \tilde{r} & \alpha_3 r_2 r_4 \sin \theta_{24} \\
\alpha_3 r_2 r_4 \sin \theta_{24} & -\alpha_3 r_2 r_4 \cos \theta_{24} + \mu_3 + \tilde{r}
\end{bmatrix}
\begin{bmatrix}
x_3 \\
y_3
\end{bmatrix},
\] (4.20)

where \( \tilde{r} = e_{32} r_2^2 + e_{33} r_3^2 + e_{34} r_4^2 \), and \( \theta_{24} = \theta_2 + \theta_4 \). The linearization of (4.18)–(4.20) at the mixed mode \( r_2 = \hat{r}_2, r_3 = 0, r_4 = \hat{r}_4, \phi_2 = \pi, \phi_4 = \pi \), yields, in the mixed-mode representation \((r_2, x_3, y_3, r_4, \phi_2, \theta_{24})\), the following matrix

\[
\begin{bmatrix}
\mu_2 + 3 e_{22} \hat{r}_2^2 + e_{24} \hat{r}_4^2 - \hat{r}_4 & 0 & 0 & 2 e_{24} \hat{r}_2 \hat{r}_4 - \tilde{r}_2 & 0 & 0 \\
0 & \hat{\mu}_3 + e_{32} \hat{r}_2 \hat{r}_4 \cos \theta_{24} & \hat{\mu}_3 - e_{32} \hat{r}_2 \hat{r}_4 \sin \theta_{24} & 0 & 0 & 0 \\
0 & \hat{\mu}_3 - e_{32} \hat{r}_2 \hat{r}_4 \sin \theta_{24} & \hat{\mu}_3 + e_{32} \hat{r}_2 \hat{r}_4 \cos \theta_{24} & 0 & 0 & 0 \\
2 e_{42} \hat{r}_2^2 \hat{r}_4 - 2 e_{44} \hat{r}_2 & 0 & 0 & \mu_4 + e_{44} \hat{r}_2^2 + 3 e_{44} \hat{r}_4^2 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 \hat{r}_4 + \frac{\hat{r}_2^2}{\hat{r}_4} & 0 \\
0 & 0 & 0 & 0 & 0 & \hat{r}_4 + \frac{\hat{r}_2^2}{\hat{r}_4}
\end{bmatrix},
\] (4.21)

where \( \hat{\mu}_3 = \mu_3 + e_{32} \hat{r}_2^2 + e_{34} \hat{r}_4^2 \). Observe that the group action forces one eigenvalue of (4.21), in the lower block, to be zero due to the circle of mixed-mode equilibria. The other eigenvalue, in the same lower block, is \( 2 \hat{r}_4 - \frac{\hat{r}_2^2}{\hat{r}_4} \), it is associated with the branches of pitchfork bifurcation to traveling waves.

Now, stability in the \( z_3 \)-direction is determined by the eigenvalues of the \( 2 \times 2 \) block matrix formed by columns(rows) two and three of the linearization matrix (4.21). But observe first, also from (4.21), that \( \theta_{24} \) evolves according to

\[\dot{\theta}_{24} = \left( \hat{r}_4 \mp \frac{\hat{r}_2^2}{\hat{r}_4} \right) \sin \phi_2,\] (4.22)

so that \( \theta_{24} \) remains constant for the mixed mode \( \phi_2 = \pi \). Letting \( \hat{r}_4 = \rho, \hat{r}_2 = \sqrt{2} \rho \), and using (4.15), we integrate (4.22) to get

\[\theta_{24} = \mp 3 \left\{ \rho^2 - \left[ \mu_2 + \left( 2 e_{22} + e_{24} \right) \rho^2 \right] \right\}^{1/2} t + \theta_{24}(0).\] (4.23)
Without loss of generality, we set $\theta_{24} = 0$, so that the linearization becomes

$$
\begin{bmatrix}
\dot{x}_3 \\
\dot{y}_3
\end{bmatrix} =
\begin{bmatrix}
\mu_3 + (2e_{32} + e_{34})\rho^2 + \alpha_3\sqrt{2}\rho^2 \cos \omega t & \alpha_3\sqrt{2}\rho^2 \sin \omega t \\
\alpha_3\sqrt{2}\rho^2 \sin \omega t & \mu_3 + (2e_{32} + e_{34})\rho^2 - \alpha_3\sqrt{2}\rho^2 \cos \omega t
\end{bmatrix}
\begin{bmatrix}
x_3 \\
y_3
\end{bmatrix}.
$$

(4.24)

Following Campbell et al., we employ "rotating" polar coordinates $x_3 = r_3 \cos \theta_3$, $y_3 = r_3 \sin \theta_3$, and $\phi_3 = 2\theta_3 - (\theta_2 + \theta_4)$, to rewrite the linearization as follows

$$
\begin{align*}
\dot{r}_3 &= \left[\mu_3 + (2e_{32} + e_{34})\rho^2 \pm \alpha_3\sqrt{2}\rho^2 \cos \omega t\right] r_3 \\
\dot{\phi}_3 &= \omega - 2\alpha_3\sqrt{2}\rho^2 \sin \phi_2.
\end{align*}
$$

(4.25)

In a similar manner to that of the mode interaction studied by Campbell et al., Eq. (4.25) indicates that the traveling wave at $z_3 = 0$ is "blown-up" in the radial direction $r_3$ through the circle $r_3 = 0$ while the phase difference $\phi_3$ obeys that of a classical nonuniform oscillator. That is, when $2\sqrt{2}\alpha_3\rho^2 < |\omega|$, the evolution of $\phi_3(t)$ is very slow near a bottleneck that occurs at $\phi_3 = \pi/2$ but it moves on a faster scale away from the bottleneck. When $2\sqrt{2}\alpha_3\rho^2 = |\omega|$, the oscillations in $\phi_3$ stop altogether, a half-stable fixed point emerges via a saddle-node bifurcation at $\phi_3 = \pi/2$. It is only at this isolated point that the phase difference $\phi_3$ remains constant, so that the individual phase $\theta_3$ is locked with those of $\theta_2$ and $\theta_4$. Finally, when $|\omega| < 2\sqrt{2}\alpha_3\rho^2$, the half-stable fixed point splits into two fixed points, one stable and one unstable, so that $\phi_3(t)$ is eventually attracted to the stable fixed point. Thus, attractivity in the $z_3$-direction is determined by the following two quantities

$$
\mu_3 + (2e_{32} + e_{34})\rho^2 \pm \alpha_3\sqrt{2} \left(\rho^4 - \frac{\omega^2}{8\alpha_3^2}\right). \tag{4.26}
$$

If both quantities are negative (positive) then the traveling wave within the invariant subspace $z_3 = 0$ is asymptotically stable (unstable). FIG. 4.14 shows computer simulations of the full normal forms (4.11) for the former case, i.e., the wave speed is relatively small so that $z_3$ approaches zero and the flow of the full system becomes asymptotically attracted to the traveling wave in $z_3 = 0$. 
Figure 4.14. Phase-space portraits of a traveling wave found in simulations of the normal form equations (4.11). Parameters are: \( \mu = (0.235, 0.132, 0.2) \), \( \alpha = (0, 2, 0) \), \( e_2 = (-4, 0, 0.1) \), \( e_3 = (-1.6, -1, -1.6) \), \( e_4 = (-2, 0, -2) \). \( z_3 \) approaches zero as time evolves, so the flow of the system is asymptotically attracted to the traveling wave in the invariant subspace \( z_3 = 0 \).

On the other hand, if

\[
\mu_3 + (2e_{32} + e_{34})\rho^2 - \alpha_3 \sqrt{2(\rho^4 - \omega^2/(8\alpha_3^2))} < 0 \\
\mu_3 + (2e_{32} + e_{34})\rho^2 + \alpha_3 \sqrt{2(\rho^4 - \omega^2/(8\alpha_3^2))} > 0,
\]

then the traveling wave is of saddle-type in the \( z_3 \) direction. Consequently, the traveling wave stabilizes in \( z_3 \) when the wave speed increases sufficiently that

\[
[\mu_3 + (2e_{32} + e_{34})\rho^2]^2 = 2\alpha_3^2\rho^4 - \omega^2/4.
\]

FIG. 4.15 depicts this latter case. According to (4.19) and to our previous discussion, the individual phase \( \theta_3 \) evolves non-uniformly, which can also be observed directly in
FIG. 4.15. Hence in the complete phase space \((z_2, z_3, z_4)\), the wave is, effectively, a modulated traveling wave.

\[\begin{align*}
0.4 & \quad 0.2 & \quad 0 & \quad -0.2 & \quad -0.4 \\
-0.4 & \quad -0.2 & \quad 0 & \quad 0.2 & \quad 0.4 \\
0.4 & \quad 0.2 & \quad 0 & \quad -0.2 & \quad -0.4 \\
-0.4 & \quad -0.2 & \quad 0 & \quad 0.2 & \quad 0.4
\end{align*}\]

Figure 4.15. Phase-space portrait of a traveling wave similar to that of FIG. 4.14, except that now the wave stabilizes in the \(z_3\) direction. Phase evolution in the \(z_3\) direction is non-uniformly, thus the wave in the complete normal form space \((z_2, z_3, z_4)\) is, effectively, a modulated traveling wave. Parameters are: \(\mu = (0.235, 0.135, 0.2), \alpha = (0, 2, 0), e_2 = (-4, 0, 01), e_3 = (-1.6, -1, -1.6), e_4 = (-2, 0, -2)\).

4.6.2 Modulated Traveling Waves

In the subspace \(z_3 = 0\), modulated traveling waves are periodic solutions of the polar-coordinate system (4.13) with \(\phi_2 \neq 0, \pi\). As in the \(k : 2k\) mode interaction of Armbruster et al., these waves are created via a Hopf bifurcation from the branch of traveling waves at

\[\mu_4 = \mu_2 \left[1 + \frac{9(e_{44} - e_{24})}{e - 3(e_{44} - e_{24})}\right],\]  

(4.27)
where we recall that $e = 4e_{22} + 2e_{24} + 2e_{42} + e_{44}$. They exist within the parameter region defined by

\[ \mu_2 \left[ 1 + \frac{9(e_{44} - e_{24})}{e - 3(e_{44} - e_{24})} \right] + O(\mu_2^2) < \mu_4 < \frac{e_{44}}{e_{24}} + O(\mu_2). \]  

(4.28)

To study the stability of modulated traveling waves, we re-scale the full polar system (4.18) using $r_j = \varepsilon s_j$, $j = 2, 3, 4$; $\mu_j = \varepsilon^2 \nu_j$, $j = 2, 4$; $\mu_3 = \varepsilon \nu_3$; and $() = (\cdot)'$, getting

\[
\begin{align*}
    s'_2 &= s_2 s_4 \cos \phi_2 + \varepsilon \alpha_2 s_3^2 s_4 \cos \phi_3 + \varepsilon s_2 (\nu_2 + e_{22} s_2^2 + e_{23} s_3^2 + e_{24} s_4^2) \\
    s'_3 &= \nu_3 s_3 + \varepsilon \alpha_3 s_2 s_3 s_4 \cos \phi_3 + \varepsilon s_3 (\nu_3 + e_{32} s_2^2 + e_{33} s_3^2 + e_{34} s_4^2) \\
    s'_4 &= \pm s_3^2 \cos \phi_2 + \alpha_4 s_2^2 s_4 \cos \phi_3 + \varepsilon s_4 (\nu_4 + e_{42} s_2^2 + e_{43} s_3^2 + e_{44} s_4^2) \\
    \phi'_2 &= -\left(2s_4 \pm \frac{s_2^2}{s_4}\right) \sin \phi_2 + \varepsilon \left(2\alpha_2 s_2^2 s_4 - \alpha_4 \frac{s_2 s_3^2}{s_4}\right) \sin \phi_3 \\
    \phi'_3 &= \left(s_4 + \frac{s_2^2}{s_4}\right) \sin \phi_2 - \varepsilon \left(2\alpha_3 s_2 s_4 + \alpha_2 \frac{s_2 s_3^2}{s_4} + \alpha_4 \frac{s_2 s_3^2}{s_4}\right) \sin \phi_3.
\end{align*}
\]  

(4.29)

The linearization of (4.20)–(4.29) at the traveling wave $s_4 = \rho$, $s_2^2 = \sqrt{2}\rho$, with (4.15), yields in the mixed-mode representation the same stability properties as those of the $(z_2, z_4)$ traveling wave of Armbruster et al.. That is, if $e_{44}, e_{24} < 0$ and $e < 0$, then modulated traveling waves, in $z_3 = 0$, are stable for $\mu_2 < \mu_1 a$ and unstable saddles for $\mu_2 > \mu_1 a$, where $a = [1 + 9(e_{44} - e_{24})/(e - 3(e_{44} - e_{24}))]$. Along the $z_3$-direction, the linearization leads to

\[
\begin{align*}
    \dot{s}_3 &= \left[\nu_3 + \varepsilon((2e_{32} + e_{34})\rho^2 \pm \alpha_3 \sqrt{2}\rho^2 \cos \omega t)\right] s_3 \\
    \dot{\phi}_3 &= \omega - 2\alpha_3 \sqrt{2}\rho^2 \sin \phi_2.
\end{align*}
\]  

(4.30)

It follows that modulated traveling waves at $z_3 = 0$ are also blown up into the radial direction $s_3$ through the circle $s_3 = 0$ and, as expected, the phase $\phi_3$ also evolves non-uniformly. Up to order $\varepsilon$, if $\nu_3$ is negative (positive) then the modulated traveling wave at $z_3 = 0$ is asymptotically stable (unstable). On the other hand, if $\nu_3 + \varepsilon((2e_{32} + e_{34})\rho^2 - \alpha_3 \sqrt{2}\rho^2 \cos \omega t) < 0$ and $\nu_3 + \varepsilon((2e_{32} + e_{34})\rho^2 + \alpha_3 \sqrt{2}\rho^2 \cos \omega t) > 0$ then the modulated wave is of saddle-type in the $z_3$ direction. Consequently, the modulated traveling wave stabilizes in $z_3$ when the wave speed increases sufficiently that $[\nu_3 + \varepsilon((2e_{32} + e_{34})\rho^2)]^2 = 2\alpha_3^2 \rho^2 \cos^2(\omega t)$, as is illustrated in FIG. 4.16.
Figure 4.16. Phase-space portraits of a modulated traveling wave found in simulations of the normal form equations (4.11). Parameters are: \( \mu = (0.235, 0.132, 0.35) \), \( \alpha = (0, 2, 0) \), \( e_2 = (-4, 0, 0.1) \), \( e_3 = (-1.6, -1, -1.6) \), \( e_4 = (-2, 0, -2) \).
CHAPTER 5
INTEGRATION OF THE STOCHASTIC KURAMOTO-SIVASHINSKY EQUATION; THE ADDITIVE NOISE CASE

Noise is ubiquitous to the physical world. Historically, it has been considered a nuisance to scientists and engineers who have used considerable effort to suppress it. In more recent years the constructive effects of noise have been examined. In particular, the introduction of noise in a dynamical system can result in organized behavior that does not exist in the absence of noise. An example is stochastic resonance; a phenomenon where an unobservable weak signal can be amplified by noise of the proper intensity to the point where it becomes observable [83]. Another example is the formation of stochastic limit cycles about equilibria of heteroclinic and homoclinic connections. For instance, consider the dynamics of a particle moving along a double-well potential, described by the unforced Duffing oscillator $\ddot{x} = -\dot{x} + x - x^3 + \xi(t)$, where $\xi(t)$ represents a Gaussian white noise function. In the absence of noise, i.e., when $\xi(t) = 0$, the particle will quickly settle into one of the two equilibrium states represented by the minima of the potential function, see FIG. 5.1.

In the presence of noise, however, the noise intensity might be too small to change the eigenvalues of a system, but large enough to keep the solution from approaching an equilibrium. Thus the solution will linger around an equilibrium only for finite and random amounts of time, as is now shown in FIG. 5.2.

In a spatially-extended system where the dynamics are described by the Kuramoto-Sivanshinsky equation, equilibrium points describing ordered cellular flame steady-states might have a spatial structure. In these systems, stochastic limit cycles can lead to intermittent patterns in which one or more ordered patterns appear at random intervals as the system dynamics approach a neighborhood of an equilibrium state.
Figure 5.1. Motion of a particle on a double-well potential function. In the absence of noise, the system dynamics quickly settles into an equilibrium point. Which equilibrium point is selected, (left) or (right), depends on the initial conditions.

Figure 5.2. Motion of a particle on a double-well potential function subject to noise. The system dynamics now lingers intermittently between the two equilibrium states of the deterministic system, independently of initial conditions.

In this work, we investigate the effects of noise in a stochastic version (Langevin formulation) of a generic example of a pattern-forming dynamical system, with circular domain, known as the Kuramoto-Sivashinsky (KS) equation

$$ \frac{\partial u}{\partial t} = \eta_1 u - (1 + \nabla^2)^2 u - \eta_2 \nabla u^2 - \eta_3 u^3 + \xi(x, t), $$

(5.1)

where $u = u(x, t)$ represents the perturbation of a planar front (typically assumed to be a flame front) in the direction of propagation, $\eta_1$ measures the strength of the perturbation force, $\eta_2$ is a parameter associated with growth in the direction normal to the circular
domain (burner), and \( \eta u^3 \) is a term that is added [22] to help stabilize the numerical integration, and \( \xi(x, t) \) represents Gaussian white noise, which models thermal fluctuations, dimensionless in space and time. We assume \( \xi(x, t) \) to be distributed with zero mean \( \langle \xi(x, t) \rangle = 0 \), and to be uncorrelated over space and time, i.e.

\[
\langle \xi(x, t) \xi(x', t') \rangle = 2D \delta(x - x') \delta(t - t'),
\]

(5.2)

where \( D \) is a measure of the intensity of the noise, \( \langle \cdot \rangle \) represents the time-average over a range of observations. It is observed that simulations performed in the absence of noise provide a multitude of results involving stationary states; while the inclusion of noise provides perturbation and asymmetry to the system that allows for the observance of dynamic states, previously thought to be stationary in noise free analysis.

In this chapter we build on the Crank-Nicolson based Integration scheme, described in Section 3.4, in order to study the effects of noise on the formation of cellular patterns. We observe, through computer simulations, that in the absence of noise equation 5.1 shows a greater tendency towards stationary states. In the presence of noise, the preferred patterns are, however, dynamic states. The numerical observation of certain dynamic states (previously described alternately by experimentalists as either homoclinic or heteroclinic cycles) are reported. Until now they had only been observed in laboratory experiments.

### 5.1 The Additive Noise Solver

The numerical scheme used to integrate the stochastic version of the KS model (5.1) is based on the Crank-Nicolson solver described in the prior Subsection 3.4. Here we review the properties and describe the modifications introduced to allow for the inclusion of additive noise. The scheme remains second order in time, and based on the Crank-Nicolson scheme [23], which is linearly unconditionally A-stable. In order to numerically resolve the nonlinearity, the scheme employs a Newton iteration in each time-step, in which the resulting sequence of linear systems are solved using the preconditioned Bi-CGSTAB method [122]. The preconditioner is chosen to be the unchanging linear part of the discretized operator. Converting the noisy form of the
KS-equation (5.1) to polar coordinates, suitable for the circular domain, yields

\[ u_t = -u_{rrrr} - \frac{1}{r^4}u_{\phi\phi\phi\phi} - \frac{2}{r^2}u_{r\phi\phi} - \frac{2}{r}u_{rrr} + \frac{2}{r^3}u_{r\phi} \]

\[ - \left[ 2 - \frac{1}{r^2} \right] u_{rr} - \left[ \frac{4}{r^4} + \frac{2}{r^2} \right] u_{\phi\phi} - \left[ \frac{1}{r^3} + \frac{2}{r} \right] u_r \]

\[ + \eta_1 u - \eta_2 \left[ u_r^2 + \frac{1}{r^2} u_{\phi}^2 \right] - \eta_3 u^3 + \xi(r, \phi, t). \]

Let \( \vec{x} = (r, \phi) \) and let \( F(\vec{x}, t, u(t), \xi(t)) \) represent the right-hand side of (5.1), where for convenience we suppress the dependence on \( \vec{x} \), so that \( u_t(t) = F(\vec{x}, t, u(t), \xi(t)) \). Further, for this discussion we decompose the right-hand side, \( F(\vec{x}, t, u(t)) \) into deterministic and a stochastic parts, or \( F(\vec{x}, t, u(t)) = F_{\text{det}}(\vec{x}, t, u(t)) + F_{\text{sto}}(\vec{x}, t) \), e.g.

\[ F_{\text{det}}(\vec{x}, t, u(t)) = -u_{rrrr} - \frac{1}{r^4}u_{\phi\phi\phi\phi} - \frac{2}{r^2}u_{r\phi\phi} \]

\[ - \frac{2}{r}u_{rrr} + \frac{2}{r^3}u_{r\phi\phi} - \left[ 2 - \frac{1}{r^2} \right] u_{rr} \]

\[ - \left[ \frac{4}{r^4} + \frac{2}{r^2} \right] u_{\phi\phi} - \left[ \frac{1}{r^3} + \frac{2}{r} \right] u_r \]

\[ + \eta_1 u - \eta_2 \left[ u_r^2 + \frac{1}{r^2} u_{\phi}^2 \right] - \eta_3 u^3, \]

\[ F_{\text{sto}}(\vec{x}, t, u(t)) = \xi(t). \]

Since the stochastic term is uncorrelated (white) in time, and independent of \( u(t) \), we can evaluate the term in the center of the time-step, i.e. at time \( t + \frac{h}{2} \), thus solving 3.11 using the Crank-Nicolson scheme [23] we get an equation for the unknown \( u(t + h) \)

\[ \frac{u(t + h) - u(t)}{h} = \frac{F_{\text{det}}(\vec{x}, t, u(t))}{2} \]

\[ + \frac{F_{\text{det}}(\vec{x}, t + h, u(t + h))}{2} + F_{\text{sto}}(\vec{x}, t + h/2). \]
Equation (5.5) leads to a nonlinear system of equations of the form
\[ G(u(t + h)) = 0, \]
which we solve for \( u(t + h) \) using Newton’s method as follows
\[
\vec{u}^{n+1}(\vec{x}, t + h) = \vec{u}^n(\vec{x}, t + h) - \left[ \delta \vec{G}(\vec{u}^n(\vec{x}, t + h)) \right]^{-1} \cdot \vec{G}(\vec{u}^n(\vec{x}, t + h)),
\] (5.6)
\[
\vec{u}^0(\vec{x}, t + h) = \vec{u}(\vec{x}, t).
\] (5.7)
Here \( \delta \vec{G} = \nabla_u \vec{G}(\vec{u}^n(\vec{x}, t + h)) \) is the Jacobian. Since \( F_{\text{sto}}(\vec{x}, t + h/2) \) does not depend on \( u(\vec{x}, t + h) \), it only affects the linear system as a constant addition to \( G(u(t + h)) \), with no contribution to the Jacobian. In each step of the Newton-iteration we solve the linear system
\[
\left[ \delta \vec{G}(\vec{u}^n(\vec{x}, t + h)) \right] \delta \vec{u} = \vec{G}(\vec{u}^n(\vec{x}, t + h)).
\] (5.8)
In our simulations, the grid is subdivided into \( N_r = 32 \) radial points, and \( N_\phi = 64 \) azimuthal points, leading to nearly dense \( 2048 \times 2048 \) systems. These are solved using the preconditioned biconjugate gradient stabilized method (Bi-CGSTAB) [6] described in Appendix Section B.2.
5.1.1 C Code Flow Diagram

Flow Chart for main.c
Kuramoto-Sivashinsky Crank-Nicolson Solver
with additive noise and average velocity calculation

Figure 5.3. Flow Chart for the C Code Implemented for the Additive Noise Solver.
5.2 Simulations in the Presence of Noise

Computer simulations indicate a greater tendency towards stationary states (as opposed to dynamic states) in noise-free simulations of the KS model (5.1). Stationary states are patterns with petal-like cellular structures and well-defined spatial symmetries, FIG. 5.4 illustrates a few examples. Dynamic states are patterns in which the cells move, either individually or in ring configurations.

![Representative examples of stationary states found in numerical simulations of the KS model (5.1), with $\xi(\vec{x}, t) = 0$, i.e., without noise.](image)

Figure 5.4. Representative examples of stationary states found in numerical simulations of the KS model (5.1), with $\xi(\vec{x}, t) = 0$, i.e., without noise.

As the radius of the circular domain increases, the typical ordered state that appears changes from a single ring of cells to concentric rings of cells. Occasionally, dynamic states are also observed in the transition from from one stationary pattern to another. In previous work [93], the selection mechanism behind this transition was studied; in particular, it was explained why cellular patterns consist of rings of cells and the mechanisms that lead to some dynamic states was determined. More specifically, it was found that uniformly rotating and modulated rotating single-ring states with $k$ cells were typically generated by the interaction of two steady-state modes with Fourier wave numbers in a $k : 2k$ ratio. For this reason we focus our attention around a $1 : 2$ mode interaction, though the analysis still captures many essential features of the effects of noise on larger patterns. The diagram in
FIG. 5.5 depicts the transition that results from such mode interaction. Without noise, i.e., noise amplitude $D = 0$, a one-cell rotating state (1R) appears in the transition from a one-cell stationary state to a two-cell stationary state, just as predicted by the corresponding 1:2 mode interaction.

As the noise intensity increases, the domain of existence of the 1R-state increases and additional patterns emerge, see FIG. 5.5. For very weak noise, an unsteady dynamic pattern (1U) appears between the 1S and 1R states. The 1U pattern does not sustain rotations; instead, the pattern rocks back and forth. With increased noise intensity, a one-cell rotating pattern (1RL), which intermittently changes its direction of rotation, is observed between the 1U and 1R patterns. Near the bifurcation point, where the 1RL state forms, there are two bistable branches of rotating states created by symmetry, one branch for each direction of rotation. Which branch is observed depends mainly on initial conditions. Noise appears to act as a switch, inducing recurrent transitions between these two branches. Between the 1R and 2S (or, for higher noise intensities, 2U) patterns, an intermittent 1-2 cell pattern (1-2I) forms. This dynamic pattern is very peculiar: one of the two cells in the 2S state is extinguished; the remaining one-cell state is short-lived, the pattern immediately splits into a new 2S-state, the orientation of which is roughly a quarter-rotation of the previous 2S-state. Each appearance of the 2S state lasts an irregular amount of time, ranging from a few to several hundreds of frames. This is qualitative evidence of a heteroclinic connection where the stable (unstable) manifold of a two-cell equilibrium is also the unstable (stable) manifold of another two-cell equilibrium. Until now, this pattern had only been observed in laboratory experiments [44, 116] but not in computer models. Finally, a 2-cell analogue (2U) of the 1U pattern forms between the 1-2I and 2S patterns.

5.3 Analysis of Intermittent Dynamics

Intermittent flame states were observed by Gorman et. al. to be prevalent in propane-air cellular flames [44]. In parameter space that contained these patterns, mostly disorder was observed in which there was no discernible structure. Then an the ordered
Figure 5.5. Behavior of the KS model for various parameter values of radius and noise intensity. Notation: 1 = single cell, 2 = 2 cell. S = Stationary, U = Unsteady, I = Intermittent State, R = Rotation. Noise intensity, $D = \sigma^2/2$, is in the range $[0.00, 2.5E-04]$. This range represents low noise levels, relative to the dynamic range of $u$, which in the Kuramoto-Sivashinsky equation is of order 10. As the noise intensity increases, the radius-parameter range of complex dynamic patterns is extended; when the intensity reaches $D = 1.25 \times 10^{-3}$ no static patterns are observed. For each of these simulations $\eta_1 = 0.32$, $\eta_2 = 1.0$, $\eta_2 = 0.017$, $4.1 \leq \text{radius} \leq 4.35$, and $D \leq 0.5$.

state would appear for a random period of time before vanishing as the flame returned to a disordered state. The ordered state would continue to reappear for varying lengths of time, from ten to several hundred frames. A composite image showing a variety of intermittent
Figure 5.6. Snapshots of the patterns observed in the 1 : 2 mode interaction under noisy and noise-free conditions.
flame patterns as well as the persistent ordered states which they resemble, is reprinted in FIG. 5.7. Of interest to this dissertation is row b which contains a 1-2I pattern in the center. It can be seen that the occurrence of the 2 cell state appears in a roughly 1/4 rotation orientation from the prior appearance. This relatively common experimentally observed type of spatiotemporal pattern had never before been simulated in two dimensions using the Kuramoto-Sivanshinsky Equation.

5.3.1 Mode Decomposition

In order to explain, quantitatively, the origin and formation mechanisms of the noise-induced intermittent pattern shown in FIG. 5.5, we perform next a Proper Orthogonal Decomposition [66, 73, 76, 94, 102] analysis of an ensemble, made up of about 4000 computer-simulated spatio-temporal data points (frames), for each individual case. To ensure that the POD steady-state modes contain the correct symmetry properties, special care was taken to include the average over the symmetry group, \(O(2)\), of the experiment, in the form of an ensemble average. In all four cases, the POD analysis reveals that two pairs of modes with wave numbers in a 1:2 ratio capture most of the dynamics, see FIG. 5.8. The time-average (considered mode \(\Phi_0\)) is shown first followed by four POD modes, \(\Phi_1-\Phi_4\), with the highest percentage of energy (see Appendix Section C.1 for an exact definition). The actual amount of energy in each mode is indicated below each mode. Each mode shows some amount of symmetry. The symmetry of the time-average, in particular, reflects the \(O(2)\)-symmetry of the burner, even though none of the instantaneous snapshots has this symmetry. This feature is studied in more detail in [29]. \(\Phi_1\) and \(\Phi_2\) show \(D_1\)-symmetry, while \(\Phi_3\) and \(\Phi_4\) show \(D_2\)-symmetry, i.e., the patterns are restored after half a revolution. Observe also that the energy is equally distributed among these two pairs of modes, which together capture almost 90% of the original behavior. It follows that intermittent behavior in all three cases is created from the mutual interaction of two invariant eigenspaces, \(V_1 = \text{span}\{\Phi_1, \Phi_2\}\) and \(V_2 = \text{span}\{\Phi_3, \Phi_4\}\), whose dihedral symmetries are in a 1 : 2 ratio, just as expected from direct inspection of the transition diagram of FIG. 5.5. We postpone
Figure 5.7. A composite image displaying four different intermittent patterns as well as the persistent ordered states which they resemble. Row a shows a persistent 9/1, while row b shows a pattern where the outer ring of 9 cells persists while the inner cell intermittently splits into two cells. Row c shows a persistent 9/3 while row d shows an intermittent 9/3 state. Row e shows a persistent 10/4 state, while row f shows an intermittent 10/4 state. Row g shows a persistent 11/5, while row h shows an intermittent 11/5. This image is reprinted from [44].

further discussion of the 1RI and 1U patterns until later when we compare results of the POD decomposition with solutions of the associated amplitude equations.

Next we examine results of the POD decomposition of the 1-2I intermittent state. FIG. 5.9 shows the time-dependent coefficients associated with each individual POD mode.
Figure 5.8. A proper orthogonal decomposition analysis reveals that all four patterns of FIG. 5.5 are created from the mutual interaction of two pairs of spatial modes whose wave numbers are in a 1:2 ratio. These modes were obtained using computer-simulated ensembles of 4000 data set points of each individual pattern.

To help visualize the actual transitions, we have added two markers, a green circle and a red circle. The time between the green (red) circle and the red (green) define the beginning and end of a 2-cell (1-cell) pattern, respectively. Observe that when the oscillations in \( a_1(t) \) and \( a_2(t) \) have large amplitudes relative to those of \( a_3 \) and \( a_4 \), the 1-cell pattern shows up. The opposite relation, small amplitude in \( a_1, a_2 \) and large amplitude in \( a_3, a_4 \), leads to the appearance of the 2-cell pattern.

Figure 5.9. Amplitude coefficients associated with the POD modes of the intermittent state 1-2I of FIG. 5.5. Horizontal axis denotes time. Markers indicate beginning (green) and end (red) of a 2-cell pattern.
The heteroclinic saddle-node connections that underlie the transitions between the 1-cell pattern and the 2-cell state, can be observed better in the phase-space portrait of FIG. 5.10. Black arrows indicate the approximate direction of the flow around the two saddle-nodes that are associated with a 2-cell state, while there are four saddle-nodes that correspond to the 1-cell state. This difference deserves an explanation. Once a 2-cell state appears in the simulations, there is only one distinct orthogonal position in which the same pattern can reappear. On the other hand, a 1-cell state has four orthogonally distinct positions where it can reappear. These geometric facts determine the structure of the phase portrait of FIG. 5.10.

Figure 5.10. Phase-space portrait from time-dependent POD coefficients for an intermittent state 1-2I clearly capture saddle-node connections between the stable and unstable manifolds associated with each individual ordered pattern, one with one cell and one with two cells.

The relationship between unstable equilibria and intermittent system behavior has been well described in physics literature, especially concerning turbulence. It was described as early as 1971 by Kim et al. [68]. It has been observed in the Navier-Stokes equation [2].
It has also been observed in cellular flames by Stone et al. [116]. A full review has been compiled by Holmes [57]. The theory is fully developed and will only be given a basic treatment here.

Generally speaking, an unstable saddle node equilibria has both stable and unstable eigenvalues. If a homoclinic cycle exists then there is some orbit for which as time \( t \to \infty \) the trajectory will approach the saddle and as \( t \to -\infty \) the trajectory also approaches the saddle. If a heteroclinic cycle exists, then as \( t \to -\infty \) the trajectory return to the saddle point, but as \( t \to \infty \) the trajectory approaches some other equilibrium, or vice versa. It should be noted that an equilibrium has no intrinsic time scale. Which is to say that the magnitude of the phase vectors grow asymptotically small as they are nearer to the equilibrium. Therefore if a trajectory passes arbitrarily close to an equilibrium, it slows to a quasi-stationary state. This being said, the majority of trajectories should eventually diverge from a saddle type equilibrium.

However, If the real parts of the unstable eigenvalues of a saddle node are much smaller than the real parts of the stable eigenvalues, then it can be generalized that the trajectories leave a neighborhood of the equilibrium closer to the connecting orbit than on entry. In the case of a homoclinic cycle, the trajectory will remain close to the connecting orbit, and upon passing the equilibrium another time, will have grown even closer to the connecting orbit. Over time it will grow arbitrarily close to that orbit, and therefore pass arbitrarily close to the equilibrium. Thus, it will eventually slow to the degree that it has essentially stopped. We will call this an "stable homoclinic connection" for the purpose of this explanation.

The existence of random perturbations in the system has a unique effect. As observed by Busse and Heikes [20], the addition of even a very small perturbation can introduce a time scale. As a result, the process leading to a stable homoclinic connection is destroyed, and one finds in its stead a "stochastic limit cycle" [117]. Thus the system never slows to a quasi-stationary state. Instead it is perpetually cycling round the homoclinic
connections. It will approach the equilibrium, but will never stop there. Instead it passes, spending varying periods of time within a certain epsilon neighborhood of the equilibrium before diverging and spending varying amounts of time away from the equilibrium.

Since the trajectory passes within an epsilon neighborhood (U) of the equilibrium, the passage time can be studied using a linearization about the equilibrium. It can be modeled using a simple Ornstein-Uhlenbeck process to calculate the passage times. The distribution can be shown to be

\[ P(T) = 2\lambda \Delta(T)e^{-\Delta^2(T)} \sqrt{\pi}(1 - e^{-2\lambda T}), \]  

where \( T = \) passage time, \( \Delta(t) = \delta[(\epsilon^2/\lambda)(e^{2\lambda t} - 1)]^{-1/2} \), \( \lambda \) is the most unstable eigenvalue of the equilibrium, \( \epsilon \) is the noise level and \( \delta \) is the size of the neighborhood U [117].

A stochastic limit cycle can also result from a system of heteroclinic connections. The primary difference is that there are more than one equilibria which are approached by the trajectory.

### 5.3.2 Amplitude Equations

As was mentioned before, all three intermittent patterns, 1RI, 1U, and 1-2I, emerge from the mutual interaction of two pairs of spatial modes, \( \{\Phi_1, \Phi_2\} - \{\Phi_3, \Phi_4\} \), with wave numbers in a 1:2 ratio, while the time evolution of each individual pattern is determined by the amplitude coefficients \( a_1(t) - a_4(t) \) that are associated with the spatial modes \( \Phi_1 - \Phi_4 \), respectively. The amplitude equations that govern the evolution of the time-dependent coefficients are derived from the 1-to-2 Fourier-mode interaction in a system with \( O(2) \)-symmetry, i.e., the symmetry group of rotations and reflections of the circular domain. The deterministic version of these amplitude equations in Birkhoff Normal Form has been thoroughly studied by Armbruster et al. [2]. The Langevin version below

\[
\begin{align*}
\dot{z}_1 &= \bar{z}_1 \bar{z}_2 + z_1(\mu_1 + e_{11}|z_1|^2 + e_{12}|z_2|^2) + \varepsilon \eta_1(t) \\
\dot{z}_2 &= \pm \bar{z}_2^2 + z_2(\mu_2 + e_{21}|z_1|^2 + e_{22}|z_2|^2) + \varepsilon \eta_2(t),
\end{align*}
\]

(5.10)

where \( \eta_1(t) \) and \( \eta_2(t) \) are Gaussian white noise functions, uncorrelated with zero mean and with amplitude \( \varepsilon \), has also been considered by Stone and Holmes [117] in a study of the
effects of noise on heteroclinic cycles. We will draw on their work when we study the 1-2I intermittent pattern; but we will also extend the analysis to other regions of parameter space in order to explain the evolution of the 1RI and 1U intermittent patterns. We start with the 1R pattern. According to the transition diagram of FIG. 5.5, and to the POD relative phase-angles plots of FIG. 5.12, it is reasonable to associate the temporal evolution of the 1R pattern with that of a traveling wave of the deterministic normal forms, i.e., $\eta_1 = 0$ and $\eta_2 = 0$ in (5.10). We claim that the 1RI pattern arises from noise perturbations of a traveling wave solution of the normal forms. We prove this claim next. For convenience, we let $z_j = re^{i\theta_j}$ and $\phi = 2\theta_1 - \theta_2$, so that we can rewrite (5.10) in polar coordinates

$$
\dot{r}_1 = r_1 r_2 \cos \phi + r_1 (\mu_2 + e_{11} r_1^2 + e_{12} r_2^2) + \varepsilon \eta_1(t)
$$

$$
\dot{r}_2 = \pm r_1^2 \cos \phi + r_2 (\mu_4 + e_{21} r_1^2 + e_{22} r_2^2) + \varepsilon \eta_2(t)
$$

$$
\dot{\phi} = -\left(2r_2\pm\frac{r_1^2}{r_2}\right)\sin \phi.
$$

(5.11)

Observe that the noise functions $\eta_1$ and $\eta_2$ do not appear, explicitly, in the last equation in (5.11), which governs the evolution of the phase-difference variable. We will show that noise can, however, change the evolution of the phase difference through the radial components $r_1$ and $r_2$. Consider the noise-free system: $\eta_1 = 0$ and $\eta_2 = 0$. Traveling Waves (TW) are equilibria of (5.10) in which the phase difference remains constant, though $\phi_2 \neq 0, \pi$. In physical space, TWs correspond to uniformly rotating patterns produced by evolution equations; e.g., the 1R pattern that appears in simulations of the Kuramoto-Sivanshinsky model (5.1). Following Armbruster et al., traveling waves (of the deterministic system) are created via a pitchfork bifurcation from the $\pi$-mixed mode solution ($r_1 \neq 0$, $r_2 \neq 0$, $\phi = \pi$) when $2r_1 \pm r_2^2/r_4 = 0$, and $\phi_2 = \pi$, so that they only exist in the “−” case or when $r_1^2 = 2r_2^2$. Letting $e = 4e_{11} + 2e_{12} + 2e_{21} + e_{22}$, it can be shown that TW solutions of (5.10), without noise, exist and are stable for

$$
-2\mu_1 - e\mu_1^2 + O(\mu_1^3) < \mu_2 < \mu_1 \left(1 + \frac{9(e_{22} - e_{12})}{e - 3(e_{22} - e_{12})}\right) + O(\mu_1^2).
$$

(5.12)
Consider now the noisy system. Direct calculations of the equilibria of (5.11) lead to

\[ \lambda r_2 + e r_2^3 + \sigma \eta_3(t) = 0, \]  

(5.13)

where \( \lambda = 2\mu_1 + \mu_2 \) and \( \eta_3 \) is also a Gaussian white noise function, uncorrelated with zero mean, but with amplitude \( \sigma = \sqrt{3}\varepsilon \). When \( \sigma = 0 \), Eq. (5.13) reduces to the normal form equation for the pitchfork bifurcation that underlie the birth of the TWs of the deterministic system. A more critical observation is the fact that additive white noise does not modify qualitatively the solution set of a codimension-one, perfect, pitchfork bifurcation \cite{65}. It follows that TW solutions, and their stability properties, of the noisy system (5.10) necessarily coincide with those of the deterministic, \( \sigma = 0 \), system; and Eq. (5.12) is still valid for the noisy system. But if the 1RI pattern is indeed a noise-perturbed TW, then we seem to have an apparent contradiction: how can noise change the direction of rotation of the 1RI state if noise cannot modify the qualitative properties of the pitchfork bifurcations that lead to traveling waves? To clarify this subtle issue, we need to take into account that equilibria of (5.11) are now described by a probability density function \( p(r_i, t) \). In the case of the pitchfork bifurcation (5.13), \( p(r_2, t) \) is governed by the following Fokker-Planck equation

\[ \partial_t p(r_2, t) = -\partial_r (\lambda r_2 + e r_2^3)p(r_2, t) + \frac{\sigma^2}{2}\partial_{rr}p(r_2, t). \]  

(5.14)

Traveling wave solutions are described by stationary solutions of (5.14), which, in turn, yields the stationary probability density function

\[ p_s(r_2) = N \exp \left[ \left( \frac{2}{\sigma^2} \right) \left( \lambda \frac{r_2^2}{2} + e \frac{r_2^4}{4} \right) \right]. \]  

(5.15)

Computer simulations, see FIG. 5.11, show that this function changes from single to double peaked as \( \lambda \) increases across zero. In both cases, \( \lambda < 0 \) and \( \lambda > 0 \), the location of the peaks always coincide with the steady states of the deterministic system. As predicted by theory, noise is not observed to modify the qualitative characteristics of the underlying pitchfork bifurcation. However, noise can change the probability distribution around the steady-state \( r_2 = 0 \). Assuming \( \lambda > 0 \), we notice that as noise intensity increases from zero,
the proportion of time spent by a typical solution of (5.11) around $r_2 = 0$ increases continuously until it reaches a maximum, at which time the phase-difference angle is no longer at an equilibrium, thus triggering a transition that changes the sign of the phase-difference angle, and ultimately, the direction of rotation of the wave. This cycle of events repeats itself at random time-intervals as the system dynamics in $r_2$ change back and forth between zero and the values of the deterministic system. As for the 1U pattern, since standing waves lie on the invariant subspace $\phi = 0$, or $\phi = \pi$, noise perturbations of the radial components $r_1$ and $r_2$ cannot destroy the invariance of the subspaces because they do not enter, explicitly, into the dynamics of the phase angle. Consequently, the only possible effect of noise variations in $r_1$ and $r_2$ is to create small oscillations in the phase-angle variable $\phi$, thus rocking the wave back and forth.

Figure 5.11. Stationary probability density of the radial component of the pitchfork bifurcation that leads to TW solutions.
To further verify the validity of the previous assertions, we compare in FIG. 5.12 the relative phase-angle obtained from the amplitude coefficients associated with each pair of POD modes with those from the normal form equations. The linear variation of the phase angles of the 1R pattern indicate that this pattern rotates uniformly, in which a negative slope is also indicative of counter-clockwise rotations. In the 1U state, the phase angles only jiggle back and forth since the pattern does not make any revolutions. In the 1RI pattern, however, the phase angles vary enough to induce rotations but the variations are accompanied with random changes in the direction of rotation.

![Graphs showing phase-angle variations for different patterns](image)

**Figure 5.12.** Comparison of relative phase-angles for the patterns: 1R, 1U, and 1RI, obtained from the POD analysis (left) and from the normal form equations (right).

Let’s now turn our attention to the 1-2I pattern, which brings us back to the work of Stone and Holmes [117]. Among their findings, most relevant to the analysis of the 1RI pattern, is the realization that certain intermittent states can be described as noise-induced “stochastic limit cycles” that are created from the perturbation of heteroclinic orbits connecting saddle-node equilibria of the deterministic \( \varepsilon = 0 \) normal forms. Furthermore,
the passage time of a typical orbit lingering near one of these equilibrium points obeys the following probability distribution function

\[ P(t) = \frac{2\lambda \Delta(t) e^{-\Delta^2(t)}}{\sqrt{\pi(1 - e^{-2\lambda t})}} \] (5.16)

where \( \Delta(t) = \delta[(\varepsilon^2/\lambda)(e^{2\lambda t} - 1)]^{-1/2} \), \( \lambda \) is the largest unstable eigenvalue of the equilibrium points, \( \varepsilon \) is the noise amplitude seen in (5.10), and \( \delta \) is the size of a neighborhood around the equilibrium points. In FIG. 5.13 we calculate the passage times (vertical bars) using numerical simulations of the 1-2I pattern. The equilibrium points correspond to the two different orientations of the two-cell states that appear intermittently. The bold curve is a fitting of the probability distribution function \( P(t) \) given by (5.16). It is apparent that the distribution is well approximated by the (5.16). The success of the passage time equation has already been demonstrated in reference to the actual physical experiments [116]. In an analysis of the 9/3 intermittent state, Stone et. al. were able to show the good fitting of experimental data to (5.16), see FIG. 5.14.

FIG. 5.15 depicts the phase-space projection of a typical trajectory of (5.10) onto the first two components of \( z_1 \) and the \( x \)-component of \( z_2 \), which are the analogous of the POD amplitude coefficients \( a_1, a_2 \) and \( a_3 \), respectively. The reconstructed pattern, calculated
Figure 5.14. Histogram of measured passage times $P(T)$ of the 9/3 state, using a bin size of 3, showing a comparison between the experimental results and the analytical distribution $P(T)$. Inset is an image showing a comparison between an exponential fit for a passage time histogram with a bin size of 20 frames; from the study by Stone, et al. This image is reprinted from [116].

through the following equation,

$$U_{rec}(x, t_i) = \sum_{k=1}^{4} z_k(t_i) \Phi_k(x), \quad i = 1, \ldots, M,$$

where $M$ is the size of the ensemble, 4000 frames in this case, is also shown immediately below the phase-space projection. The resemblance of the phase space with the POD phase-space projection of FIG. 5.10 is clear. More importantly, the reconstructed intermittent state is qualitatively similar, up to a rotation, to the PDE simulations. The cell rotates uniformly and, intermittently changes direction of rotation. In summary, numerical calculations, the curve fitting of $P(t)$, and the phase-space reconstruction of FIG. 5.15, are strong evidence that the 1-2I intermittent state is indeed a stochastic limit cycle created from the perturbation of a heteroclinic connection. Such connections would be unobservable under noise-free conditions.

There are two final remarks that we wish to emphasize. First, as explained earlier, more complex intermittent transitions are also found in simulations of the Langevin
Figure 5.15. Phase-space portrait from normal form equations. In comparison to FIG. 5.10 the Langevin formulation of the normal forms also display a heteroclinic connection between two 2 cell steady states. The frames below indicate the numbered points moving along the unstable manifold, to the opposite steady state, and back again along the stable manifold. There is a striking similarity in the appearance of the pattern in the normal form analysis to the pattern observed in the Kuramoto-Sivanshinsky Equation.

formulation of the KS model (5.1). For instance, FIG. 5.16 shows noise-induced intermittent behavior in a two-ring configuration, which are found in computer simulations of the Kuramoto-Sivanshinsky model (5.1) in the parameter region defined by $R = 13.101$, $D = 0.00125$, and $\eta_{1,2,3}$, as in FIG. 5.4. In principle, our analysis of the 1:2 mode interaction can be readily extended to study this more complex case of intermittency, except that the normal forms for this and many other cases have not yet been derived. The derivation of such normal forms is, however, in our plans for future work.
Figure 5.16. (Left) For $R = 13.101$, $D = 0.00125$, and $\eta_{1,2,3}$, as in FIG. 5.4, noise-induced intermittent behavior in a two-ring state is observed in computer simulations of the Kuramoto-Sivanshinskymodel 5.1. Here, the transitions visit $9/3$, $9/4$, $10/4$, and $6/3$ two-ring states at intermittent intervals. (Right) A similar multiple-ring intermittent state found in laboratory experiments. Courtesy of M. Gorman at the University of Houston.

Second, noise causes a shift in the propagation velocity of the cellular reactive front. Holding all other parameters constant, while the intensity of noise increases, we measured an increase in the angular velocity of the resulting rotation as is shown in FIG. 5.17.
Figure 5.17. Angular velocity in single cell rotations measured in radians/second as a function of noise intensity. Each line represents a series of simulations in which all parameters were held constant except for noise intensity.
CHAPTER 6
CONCLUSION AND FURTHER RESEARCH

Improvements to the Kuramoto-Sivanshinsky Integration Scheme have opened the door to further study of the physical phenomenon of cellular pattern formation. Due to symmetry arguments, the knowledge gained in the study of premixed laminar flame fronts can be applied to biological, chemical, and purely physical systems that exhibit cellular patterns through the activator-inhibitor mechanism described first by Turing [121].

The robust new Crank-Nicolson based solver shows great improvement over the prior best effort by avoiding linearizations in time, and solving the fully nonlinear problem. This improvement has been shown analytically, through a Taylor's expansion of both schemes, and practically through the ability to generate long simulations even in the presence of complex and dynamic patterns. A significant early result includes the first simulation of the hopping state, an unique dynamic pattern which had only been observed in laboratory experiments. The simulation was shown to be in good agreement with the actual physical experiment through a bifurcation analysis applying the Proper Orthogonal Decomposition and Method of Snapshots. In order to generalize the pattern to other systems, Birkhoff Normal Form equations were derived from the hopping pattern. This will allow for the study of the interaction of 3 different steady states, and can be applied to the biological, chemical, and physical systems mentioned earlier.

The inclusion of additive noise in our numerical simulator represents a further improvement in two ways. It better approximates the laboratory experiments by modeling thermal fluctuations known to occur [31]. It also provides the computational scheme necessary to study the improved model. Paramount is the observation that the occurrence of dynamic patterns as results of simulation was increased from 4% of the range studied to over 60%. This is a better comparison to the physical experiments in which very few
stationary states were seen. In fact, one could argue that no stationary states were seen in experiments; instead the highly organized patterns better resemble the unsteady patterns found in the additive noise study.

Early results from the improved solver include the first simulations of intermittent dynamics in the two dimensional Kuramoto-Sivanshinsky Equation. The 1-2I pattern has been seen in the physical experiments [44] at the base of our study, and was predicted through a study of additive noise using a normal form analysis [2]. A study of the intermittent dynamics of the pattern reveal that the passage time distribution is in good agreement with the expectation from the normal form analysis. Thus the new solver is able to simulate the heteroclinic connections that were observed in experiments, but never observable in the deterministic formulation of the Kuramoto-Sivanshinsky. The 1RI and 1U patterns are revealed to be examples of a noisy traveling wave, and a noisy standing wave respectively. A study applying the Proper Orthogonal Decomposition reveals characteristics in good agreement with bifurcation analysis from the study of complex systems.

Still the greatest achievement of this dissertation is that we have opened the door for further analysis. The parameter range in which simulation is possible is much larger than the range that has been studied. Indeed, only the radius and noise level have been adjusted in each study leaving the dimensions provided by $\eta_1$, $\eta_2$, and $\eta_3$ unexplored. It would please the author greatly to know that others would continue to research this area using these solvers. Further research could, and should continue in the following areas:

1) It is known that thermal back conduction occurs in burner flames where the burner heats up over time, leading to a preheating of the reactant. Although the physical experiment attempted to cool the burner, it is possible that a certain amount of thermal back conduction still effected the experiments. In attempt to better simulate the experiment, thermal back conduction could be modeled using a coupling to the heat equation. It is unknown what effects are caused by the phenomenon, therefore even if the
experimental counter measures proved sufficient, a study of thermal back conduction would still lead to novel results.

2) Within the deterministic model there is still a variety of opportunity to improve our understanding of cellular pattern formation. The case of multiple ring dynamics has yet to be studied. Counterrotations and Ratcheting are examples of interesting multiple ring spatiotemporal patterns that have not been fully studied. Also a more extensive study of Pulsating flame patterns and Traveling Wave flame patterns would improve the body of knowledge. These are unique dynamic states that have yet to be simulated in two dimensions.

3) A larger, more extensive study of intermittency in the Kuramoto-Sivanshinsky can help to develop the understanding of bifurcations in Complex Systems. The characteristics of a system undergoing Hopf bifurcations, for example, is currently an area of research. They, and other bifurcations occur in the system described by the Additive Noise study, and are ripe for study. Additionally, intermittency should be studied in the case of noise induced direction switching in a modulated traveling wave. This pattern has been observed in the normal form equations, but not yet in our simulations.

4) It is known that the inclusion of additive noise should not change the locations of the bifurcation points for pitchfork bifurcations. Using the Radius as an ordering parameter appears inappropriate for the Kuramoto-Sivanshinsky. Sivashinsky himself recognized the flame front velocity as the appropriate ordering parameter, and provided an equation to determine it, given in this dissertation at the end of Section 2.2.2. Preliminary investigations have shown that the integral of the state $u(x, t)$ succeeds as an ordering parameter as well. An investigation should be performed to identify the proper method, and determine how well it can be applied to other similar cellular pattern forming systems. This work should additionally include further efforts to quantify the effects of noise on the flame front velocity.

5) There are a number of other types of noise that could be studied in the Kuramoto-Sivanshinsky. Multiplicative noise is known to more greatly effect the position of
bifurcation points, and may lead to the simulation of other, or different intermittent flame dynamics. Since combustion occurs at different rates across the flame front, it may be physically justifiable to consider multiplicative noise. While it is difficult to compare characteristics of disorder, it can be said that the disorder observed in the physical experiments was prone to involve multiple rings, something rarely seen in the additive noise study. Also noise that is colored in time may allow for the greater appearance of periodic states. It too provides different effects to bifurcation points, and may induce additional dynamics.

6) There is tremendous potential in attempting to describe the bifurcations occurring in other systems using the findings of the improved numerical solvers. For instance, it may be beneficial to attempt to describe systems such as the variability in number of cotyledons formed by conifer embryos [50]. Perhaps the case of the “mutation” seen in FIG. 2.6 could be analyzed to determine if the addition of noise could shift the bifurcation point enough to allow for cotyledon production.
BIBLIOGRAPHY


APPENDIX A
REVIEW OF EXPERIMENTAL RESULTS
REVIEW OF EXPERIMENTAL RESULTS

Combustion experiments were conducted by M. Gorman, among others, at the University of Houston [46]. A description of the physical implementation is contained in this dissertation in Section 2.3 along with the current naming convention.

A.1 Steady Flame States

The simplest cellular flame state that we can describe are the Steady Flame States, see FIG. 2.7. In these states, a fixed number of cells exist, regularly distributed about the burner. These cells may fluctuate slightly in intensity or shape, but for the most part remain in a fixed position with a constant (characteristic) dimension [43]. It was been observed that the simplest steady patterns exist for low flow velocities, while higher flow velocities exhibit a higher number of cells. While experimenting with isobutane-air and propane-air mixtures, Michael Gorman et. al. were able to produce single ring steady cellular flames only when the pressure of the system was reduced to 1/3 atmosphere. The lowest number of cells produced was 5. After raising the pressure to 1/2 atmosphere, the lowest number of cells observed was 7, appearing in a 6/1 (outer ring/inner ring) orientation. Considerable effort was made to find a 7 cell single ring state, but it was never found. In the same study, much larger assemblies of steady cells were observed including a 13/6/1 state.

The experiment describes the ordered flame states by stating that the light intensity from each cell is not steady. Instead, it is chaotic. Also, some of these steady patterns exist only for brief periods of time. The pattern shown in FIG. 2.7 box k existed for only 1/30 second before the boundary evened out, and the number of cells was reduced. There was a critical flow rate that was observed, beyond which only dynamic states were observed, though that flow rate was not explicitly stated.
A table of experimental parameters resulting in the ordered states shown in FIG. 2.7. An asterisk indicates experiments run at a pressure of 1/3 atm; all others were run at 1/2 atm. The letter I indicates isobutane fuel, and the letter P indicates propane fuel. The units of flow rate are lit/min and the units of flow velocity are cm/sec. This image is reprinted from [43].

**A.2 Rotating Flame States**

The first observations of polyhedral flames, by Smithells and Ingle in 1892, involved a rotation. It was reported that “The inner cone presents a peculiar appearance. It is divided into several (usually five or six) petal-like segments, which often revolve with great rapidity round a vertical axis. [114]” Many subsequent observations of rotations were made throughout the years in the study of cellular flames, including Markstein book in 1964 [79].

Rotations, or rigid rotations, are characterized by a constant velocity periodic motion of cells around the center of the burner. The flame cells should maintain a certain shape throughout the rotation, which is to say that this state is characterized by a constant velocity periodic motion, and little or no change in shape. Rotations may involve one or more cells. In some cases a rotation may take place on only one ring in a multi-ring pattern. Sometimes multiple rings in the same pattern will rotate in the same direction, called a corotation, while in other cases rings may rotate in opposite directions, called a counterrotation. In either case, both rings commonly have the same period. The direction of rotation depends on initial conditions, and noise.

<table>
<thead>
<tr>
<th>Figure 1</th>
<th>Total flow</th>
<th>Flow velocity</th>
<th>Equiv. ratio, $\Phi$</th>
<th>Type of fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Steady</td>
<td>5.40</td>
<td>3.55</td>
<td>2.08</td>
<td>I</td>
</tr>
<tr>
<td>b) 5 cells*</td>
<td>4.52</td>
<td>2.97</td>
<td>2.21</td>
<td>I</td>
</tr>
<tr>
<td>c) 6 cells*</td>
<td>4.81</td>
<td>3.16</td>
<td>2.21</td>
<td>I</td>
</tr>
<tr>
<td>d) 1 inner</td>
<td>5.61</td>
<td>3.69</td>
<td>2.03</td>
<td>I</td>
</tr>
<tr>
<td>e) 2 inner</td>
<td>6.49</td>
<td>4.27</td>
<td>1.85</td>
<td>P</td>
</tr>
<tr>
<td>f) 3 inner</td>
<td>7.35</td>
<td>4.83</td>
<td>1.85</td>
<td>P</td>
</tr>
<tr>
<td>g) 4 inner</td>
<td>8.20</td>
<td>5.39</td>
<td>1.85</td>
<td>P</td>
</tr>
<tr>
<td>h) 5 inner</td>
<td>7.33</td>
<td>4.82</td>
<td>2.03</td>
<td>I</td>
</tr>
<tr>
<td>i) 6 inner</td>
<td>8.04</td>
<td>5.29</td>
<td>2.06</td>
<td>I</td>
</tr>
<tr>
<td>j) 7 inner</td>
<td>9.16</td>
<td>6.03</td>
<td>2.11</td>
<td>I</td>
</tr>
<tr>
<td>k) 12 inner</td>
<td>10.10</td>
<td>6.64</td>
<td>2.09</td>
<td>I</td>
</tr>
<tr>
<td>l) transient</td>
<td>11.20</td>
<td>7.36</td>
<td>2.07</td>
<td>I</td>
</tr>
</tbody>
</table>
Experimental observations by Micheal Gorman et al. [46], reported in 1994, recorded actual rotating flame states on VHS video. Their results, shown below in FIG. A.2, include examples of a single ring rotation (6R), outer ring rotation (6R/1), fixed outer ring with central ring rotation (10/2R), and two counter rotating rings (6R/2CR). You may notice in their notation that they denote clockwise rotations with a superscript asterisk, and counter clockwise rotations with a subscript asterisk.

![Figure A.2](image)

**Figure A.2.** Four examples of rotating states observed in laboratory experiments, including a single ring of six rotating cells (6R) (a), a two ring system of five cells rotating about a single cell (5R/1) (b), a system of ten stationary cells surrounding two rotating cells (10/2R) (c), and a counterrotating system with six cells rotating clockwise surrounding two cells that are rotating counterclockwise (6R/2CR) (d). This image is reprinted from [46].

Experimentally, rotating patterns are not very common, and in fact the rotations shown in FIG. A.2 columns a,c, and d did not consistently result under identical
A.3 Modulated Rotating Flame States

Modulated rotations differ from other rotations in that they involve the additional characteristics of periodic shape fluctuations and/or periodic angular velocity fluctuations during the rotation. These fluctuations may not be apparent to the naked eye, and most often require a pattern decomposition to expose.

The group at the University of Houston, lead by Michael Gorman, described a 5 cell modulated rotation. In this example, the rotation required 50 frames to complete a revolution, while its angular velocity and shape fluctuated every $3 \frac{1}{3}$ frames. The pattern is reprinted in FIG. A.4 in which a single black dot indicates the leading edge of a certain flame cell.

The category of modulated rotations encompass a variety of unique dynamical states, like ratcheting flame states and hopping flame states. However, in those cases, their unique temporal and spatial characteristics has lead to their individual study. Many modulated rotations experience velocity and shape changes that do not exhibit the particular characteristics of those types of dynamic states. These are simply classified as modulated. An example is shown in FIG. A.4.
A.4 Ratcheting Flame States

Ratcheting flame states are characterized by a periodic rotation that occurs through an nonconstant angular velocity. They can be easily distinguished from rotating flame states because the speed of rotation is always at least 2 orders of magnitude smaller. This is to say, in experiments, rotations have a minimal angular speed of 100 degrees per second, while ratcheting states have a maximal angular speed of about 1 degree per second [42].

Ratcheting motion may occur in a single ring, for example see FIG. A.5 column c. In this pattern the outer ring moves very slowly, and then briefly speeds up. Ratcheting may also occur in systems with two rings. They may corotate as in column a of FIG. A.5, or...
counter rotate as in column b. A plot of their angular displacement would show a periodic fluctuation as in FIG. A.6. Both of these figures are being reprinted from [42].

**A.5 Standing Wave Flame States**

Standing wave flame states are among the least described flame states. Fortunately one was subjected to a Proper Orthogonal Decomposition in 1999 [94]. In this example, two cells periodically split and form two new cells at roughly a 90 degree shift in position. These states are distinguishable from other dynamical states by their periodic splitting and reforming of cells. They are distinguished from intermittent states because the pattern never is in disorder, and has periodic dynamics as averse to irregular dynamics. The example is reprinted in column d of FIG. A.7.
A.6 Hopping Flame States

A special type of non-uniformly traveling wave patterns are called hopping states in which individual cells sequentially make abrupt changes in their angular positions. These type of dynamic states appear in both single-ring and multiple-ring configurations. They have been observed only in isobutane-air flames but not in propane-air flames. FIG. A.8 depicts four different configurations of hopping states. In (a) and (d), hopping occurs in a single ring array of cells, while in (b) and (c), an inner ring of hopping cells is surrounded by a stationary outer ring.

Cells in hopping states evolve collectively like rotating waves, yet individually, their motion appears more complicated and very different from other types of traveling wave patterns found in experiments [94]. Each cell seems to hop independently while still preserving the overall dynamics of the ring. That is, there is a timing rhythm for each cell to move faster and to slow down. Closer observation also reveals that when a cell is hopping, its shape is more asymmetric than the other cells which appear temporarily stationary. The characteristic that the hop occurs in a single cell at one time, rather than across all cells at the same time, distinguishes this dynamic state from modulated rotations [7].

FIG. 4.1 is an image provided by Gorman et al. [45]. It displays the four examples of hopping in a central ring (a), hopping in the middle ring (b), hopping in the outer ring (c),
Figure A.7. Four sequential frames of video tape of four different experimental flame states, including a single rotating cell (1R) (a), two rotating cells (2R) (b), counterrotating rings of six cells around two cells (6R/2CR) (c), and a standing wave between two cells. This image is reprinted from [94].

and hopping in the outer ring about a single cell(d). This group, at the University of Houston, observed a wide variety of hopping patterns leading to the belief that, at least experimentally, hopping states are relatively prevalent. The experimental data collected from the three cell hopping state shown in column a of FIG. A.8 was used as the basis for our study, and subsequent simulation of a three cell hopping state [92, 11, 12, 13].

A.7 Pulsating Flame States

Pulsating flame states are characterized by a periodic expansion and contraction of cells. These cells may also change in position or in number in a nonperiodic fashion.
Figure A.8. Four sequential frames of videotape from four experimental states with hopping motion in (a) a single ring with three cells; (b) an inner ring with three cells surrounded by a stationary outer ring with eleven cells; (c) an inner ring with two cells surrounded by a stationary outer ring with ten cells; (d) a single ring with four cells.

Pulsating flame states are found only at the boundary at the onset of cellular instability. They have been found in isobutane-air flames [44].
Figure A.9. A composite image showing an example of a stationary cellular flame (9/1) (c), and a pulsating two ring state (6P/1P) (b), and a pulsating single cell state (1P) (a). This image is reprinted from [44].

FIG. A.9 shows three different time series from a group of experiments performed by Micheal Gorman et al. The first row shows 5 time steps from an experiment in which a 9/1 pattern is unsteady. After decreasing the flow rate, the pulsating pattern shown on the second row results. In this pattern, a single cell is surrounded by 7 cells (frame 1), which contract into 6 smaller cells (frame 4), before expanding into 6 large cells (frame 5). On further decreasing the flow rate, a single cell pulsating pattern results. In this case, the planar flame front begins across the entire surface of the burner. It periodically contracts to the center of the burner, and then expands once again to cover the entire burner.

A.8 Intermittent Flame States

Intermittent flame states are characterized by a disordered flame state in which an ordered state appears and remains for an irregular amount of time, before the flame once again becomes disordered. In experiments the ordered state remained for an average of 2 seconds, but could remain for hundreds of seconds. Between ordered states, the disordered state did not hold an obvious resemblance to the ordered state. FIG. A.10 displays an image produced by Michael Gorman’s group in 1993. 15 frames depict the disordered state
occurring between two occurrences of an 11/3 ordered state. It was reported that in some cases the ordered states that appeared intermittently contained rotating dynamics or other dynamics.

![Figure A.10. Fifteen sequential frames from a video tape showing the intermittent 11/3 mode in which an ordered state vanishes in frame 2 and reappears in frame 15 at a different orientation. The 13 frames shown in between appearances of the ordered state were selected from the 112 frames that were recorded between the states to display the irregular nature of the disorder observed between ordered states. This image is reprinted from [44].](image)

At this time it was already known that intermittent dynamics represent homoclinic or heteroclinic connections between states. Three years earlier Emily Stone and Philip Holmes
had written a seminal work on the topic in which the formula for the distribution of passage
times was determined for this type of intermittent dynamics. The underlying mathematics
and derivation of the passage time formula is given later in Appendix Section B.2.

This behavior was revisited by the group, joined this time by Emily Stone, in
1994 [116]. In the second study, a heteroclinic intermittent state was observed in which 9/3,
9/4, 10/3, and 10/4 ordered states existed. In this experiment the 9/3 state appeared more
commonly than the other 3 states, and thus was the focus of the study. Passage times were
calculated by counting the number of frames in which the 9/3 ordered state was present
during a two hour time period. The experiment was performed on a propane-air flame
burning at a pressure of 1/2 atmosphere with a flow rate of 8.27 liters/min, and equivalence
ratio of 1.85. This flow rate is just beyond the flow rate at which the 9/3 steady flame state
is stable. The result was a distribution of passage times that had an exponential tail shown
in FIG. 5.14. The eigenvalue of the unstable eigenvector was found to be the inverse of $70 \\pm 2$. 

APPENDIX B
FOUNDATIONAL NUMERICAL METHODS
FOUNDATIONAL NUMERICAL METHODS

Various numerical methods were relied on for the results given in this dissertation. In this appendix we describe the properties and give the templates for the primary methods that were used.

B.1 The Crank-Nicolson Algorithm

The Crank-Nicolson Algorithm is an implicit finite difference algorithm[23]. It is used to integrate a partial differential equation (PDE) of the form $u_t = F(x, t, u)$ where $u(x,t)$ represents the spatial state of the system at time $t$. It is written as

$$
\frac{u(t + h) - u(t)}{h} = \frac{F(x, t, u(t)) + F(x, t + h, u(t + h))}{2},
$$

(B.1)

where $h$ represents the length of the step being made in time. Notice that the value of the state at time $t+h$, $(u(x,t+h))$, is not known initially. Instead an initial guess is used for $u(x,t+h)$, usually being simply $u(x,t)$, and successive approximations for $u(x,t+h)$ are made using some iterative solver. It is has been shown that the Crank-Nicolson scheme has an error of $O(\Delta x^2 + \Delta t^2)$ [98, 118].

The Crank-Nicolson scheme can be shown to be unconditionally stable through a Linear von Neumann Analysis. Von Neumann analysis is an application of Fourier analysis devised to study the stability properties of finite difference schemes. To linear order it applies to systems of equations

$$
\frac{\partial}{\partial t} \tilde{y} = L\tilde{y},
$$

(B.2)

where $L$ is a matrix capturing the finite difference (possibly in DAF representation) of spatial derivatives of $\tilde{y}$. After an appropriate change of basis, using the unitary Schur factorization $QTQ^* = L$, we can express (B.2) in transformed coordinate $\tilde{y} = Q^*\tilde{y}$

$$
\frac{\partial}{\partial t} \tilde{y} = T\tilde{y}
$$

(B.3)
where $T$ is upper triangular, with $T_{ii} = \lambda_i$. We can now limit our study to scalar equations

$$\frac{\partial}{\partial t} y = \lambda y$$

(B.4)

and note that if $\text{Re}(\lambda) < 0$, then $\lim_{t \to \infty} y(t) = 0$. Now, we integrate (B.4) in time using the Crank-Nicolson scheme

$$\frac{y^{(n+1)} - y^{(n)}}{dt} = \frac{\lambda}{2} \left[ y^{(n+1)} + y^{(n)} \right],$$

(B.5)

which, with $\hat{\lambda} = \lambda \cdot dt$, gives

$$y^{(n+1)} = \begin{bmatrix} 1 + \frac{\hat{\lambda}}{2} \\ 1 - \frac{\hat{\lambda}}{2} \end{bmatrix} g_{\text{CN}}(\hat{\lambda}) y^{(n)}.$$

(B.6)

Here $g_{\text{CN}}(\hat{\lambda})$ is the amplification factor for the Crank-Nicolson scheme. The region of absolute stability for an integration scheme is defined in terms of the amplification factor

$$R_A = \left\{ \hat{\lambda} \in \mathbb{C} : |g(\hat{\lambda})| < 1 \right\},$$

(B.7)

i.e. all the values of $\hat{\lambda}$ for which $\lim_{n \to \infty} y^{(n)} = 0$. If $R_A \supseteq \{ \hat{\lambda} : \text{Re}(\hat{\lambda}) < 0 \}$, then the method is said to be A-stable. From (B.6) it immediately follows that

$$R_{A}^{CN} = \left\{ \hat{\lambda} \in \mathbb{C} : |g(\hat{\lambda})| < 1 \right\},$$

so that the Crank-Nicolson integration is unconditionally A-stable, independent of the time-step $dt$.

### B.2 The BiCGStab Algorithm

When numerically solving the prototypical linear algebra problem, $Ax = b$, either direct or iterative methods must be used. Direct methods include the LU decomposition, and $LDL^T$ decomposition among others. They take advantage of the structure of the matrix $A$ to decompose it into a more manageable, easily invertible group of matrices. Unfortunately they quickly become impractical when $A$ becomes large, is stiff, or is sparse. Iterative methods work by solving an approximate solution, and then repeatedly solving to find a better solution until a solution is found that is good enough. Iterative methods are classified as either Stationary Methods or Nonstationary Methods[6].
Stationary methods include the Jacobi, Gauss-Seidel, Successive Overrelaxation (SOR), and Symmetric Successive Overrelaxation (SSOR) methods. They are the oldest and best known iterative methods, and can be written in the form

\[ x^{(k)} = Bx^{(k+1)} + c, \]  

(B.8)

where neither B nor c depend on the iteration count \( k \). In general, convergence of these methods is slow.

Faster convergence can be attained through nonstationary methods, and so we focus on them. Nonstationary methods differ in that the system to be solved changes in each iteration. Usually the change results from a computation using the residual of the prior iteration. Nonstationary methods include the Conjugate Gradient (CG), Minimum Residual (MinRes), Biconjugate Gradient Stabilized (BiCGStab), among others.

**B.2.1 The Conjugate Gradient Algorithm**

The Conjugate Gradient method is a well known nonstationary method, and is effective when \( A \) is symmetric positive definite. It proceeds through a series of approximations, residuals, and search directions used in prior iterations. This provides the benefit that when many iterations are required, only a few vectors must be stored in the memory. Each iteration requires the calculation of two inner products to provide values for scalars used to minimize the distance from the true solution. The method can be found in many textbooks [86, 40, 6] or through an adaptation of the preconditioned algorithm appearing in FIG. B.1. To adapt that algorithm simply removing the “solve” line, and substituting \( z^{(i-1)} \) with \( r^{(i-1)} \) (and \( z^{(0)} \) with \( r^{(0)} \)).

**B.2.1.1 Preconditioning**

The rate of convergence for the CG and most other iterative methods depends on the power spectrum of \( A \), also known as the condition of \( A \). To speed convergence, the \( A \) matrix may be transformed by another matrix called a preconditioner prior to searching for a
solution. A well chosen preconditioner will improve the convergence rate enough to justify
the cost of its construction, while assuring that the solution has not changed. Sometimes a
single preconditioner can be used repeatedly, allowing for the amortization of its cost. Often
their application allows for convergence that could not have occurred in their absence. To
introduce a preconditioner, a matrix M is found that approximates A and has favorable
invertibility properties. Then the following transformation of the system is made;

\[ M^{-1}Ax = M^{-1}b. \]  \hspace{1cm} (B.9)

In order to apply a preconditioner to the conjugate gradient method, however, the result of
the transformation must be symmetric positive definite, a quality that \( M^{-1}A \) would not
have. Instead, the matrix M is made to be symmetric, and decomposed such that
\( M = M_1M_2 \) where \( M_1 = M_2^T \). Then the transformation takes on the following form;

\[ M_1^{-1}A M_2^{-1}(M_2x) = M_1^{-1}b. \]  \hspace{1cm} (B.10)

In this case \( M_1 \) and \( M_2 \) are called left and right preconditioners, respectively.

It appears that all nonstationary iterative solvers can be preconditioned, as several
methods have been devised to generically convert an algorithm to one that contains a
preconditioner \([6, 40, 3]\). Most stationary solvers can be used as preconditioners for
nonstationary methods. Simple choices of preconditioners are the Jacobi, and SSOR
preconditioners. In other cases the results of an incomplete factorization are used, as in the
incomplete Cholesky factorization, incomplete LU factorization, or incomplete LQ
factorization. The template for the Preconditioned Conjugate Gradient algorithm is given in
FIG. B.1.

It is very similar to the original CG except for the addition of a solve step and a new
vector called \( z \). The solve step should require minimal work as M has been chosen for its
ease of inversion. In the case of a static choice for M, \( M^{-1} \) may also be found once and
stored for reuse, to reduce steps.
Compute $r^{(0)} = b - Ax^{(0)}$ for some initial guess $x^{(0)}$.

for $i = 1, 2, \ldots$

solve $Mz^{(i-1)} = r^{(i-1)}$

$\rho_{i-1} = r^{(i-1)^T}z^{(i-1)}$

if $i = 1$

$p^{(1)} = z^{(0)}$

else

$\beta_{i-1} = \rho_{i-1}/\rho_{i-2}$

$p^{(i)} = z^{(i-1)} + \beta_{i-1}p^{(i-1)}$

endif

$q^{(i)} = Ap^{(i)}$

$\alpha_i = \rho_{i-1}/p^{(i)^T}q^{(i)}$

$x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$

$r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$

check convergence; continue if necessary

end

Figure B.1. The Preconditioned Conjugate Gradient (CG) Algorithm, reprinted from [6].

### B.2.2 The Generalized Minimum Residuals, the Biconjugate Gradient, and the Conjugate Gradient Squared Algorithms

The CG method is only applicable to symmetric positive definite matrices. When the $A$ matrix is not symmetric, there is no guarantee that the update vectors will be orthogonal. For this reason, additional care must be taken when choosing an update. In order to solve the problems either the Generalized Minimum Residual (GMRES) or the Biconjugate Gradient (BiCG) methods can be used. A primary difference between the two is that GMRES solves for the inverse of $A$ through an Arnoldi Iteration, using orthonormal Arnoldi vectors. In a nutshell, the Arnoldi iteration solves for an orthogonal matrix $Q$ such that

$$ Q^T AQ = H, \quad (B.11) $$

where $H$ is the Hessenberg reduction. The Arnoldi Iteration has been described as a modified Gram-Schmidt orthogonalization applied to the Krylov sequence $A_k p^{(0)}$. The BiCG relies on Lanczos vectors, and is solving the Unsymmetric Lanczos Tridiagonalization (ULT).
The slight difference is that the ULT calculates the columns of Q as well as the rows of P such that

\[ P^T Q = I_n, \]  

(B.12)

and

\[ P^T A Q = T, \]  

(B.13)

where T is tridiagonal [40].

GMRES maintains the orthogonality of its updates by storing all of the prior q vectors. Storing this much data may become problematic, and so in practice these algorithms may be restarted after a number of iterations. It has been suggested that restarts should be put off for as large a number of iterations as possible. Without restarts, GMRES is guaranteed to converge in n steps. GMRES can be aided thought the use of a preconditioner. If ill conditioning of A cannot be avoided, householder transformations can help to improve the convergence, but at a cost of additional work per iteration. The algorithm is shown in FIG. B.2 for reference.

The BiCG maintains orthogonality of residuals by providing two mutually orthogonal sequences. One is based on the matrix A as in the conjugate gradient, the other is based on \( A^T \). This method is based on theory developed from the unsymmetric Lanczos process and is known to have irregular convergence as a result. A preconditioner can be applied to this algorithm. For reference the Preconditioned BiCG algorithm is given in FIG. B.3.

More specifically, in the BiCG the i\(^{th}\) iterate residual \( r^{(i)} \) can be described as the product of \( r^{(0)} \) and an i\(^{th}\) degree polynomial in A, or

\[ r^{(i)} = P_i(A)r^{(0)}, \]  

(B.14)

The Conjugate Gradient Squared (CGS) algorithm attempts to converge faster by multiplying that polynomial into \( r^{(0)} \) a second time, solving for \( P_i^2(A)r^{(0)} \). One result is
\( x^{(0)} \) is an initial guess

for \( j = 1, 2, \ldots \)

Solve \( r \) from \( Mr = b - Ax^{(0)} \)

\( v^{(1)} = r/\|r\|_2 \)

\( s := \|r\|_2 \epsilon_1 \)

for \( i = 1, 2, \ldots, m \)

Solve \( w \) from \( Mw = Aw^{(i)} \)

for \( k = 1, \ldots, i \)

\( h_{k,i} = (w, v^{(k)}) \)

\( w = w - h_{k,i}v^{(k)} \)

end

\( h_{i+1,i} = \|w\|_2 \)

\( v^{(i+1)} = w/h_{i+1,i} \)

apply \( J_1, \ldots, J_{i-1} \) on \( (h_{1,i}, \ldots, h_{i,i}) \)

construct \( J_i \), acting on \( i \)th and \( (i+1) \)st component

of \( h_{i,i} \), such that \( (i+1) \)st component of \( J_ih_{i,i} \) is 0

\( s := J_is \)

if \( s(i+1) \) is small enough then (UPDATE(\( \bar{x} \), \( i \)) and quit)

end

UPDATE(\( \bar{x} \), \( m \))

check convergence; continue if necessary

end

In this scheme UPDATE(\( \bar{x} \), \( i \)) replaces the following computations:

Compute \( y \) as the solution of \( Hy = \bar{s} \), in which

the upper \( i \times i \) triangular part of \( H \) has \( h_{i,j} \) as its elements (in least squares sense if \( H \) is singular),

\( \bar{s} \) represents the first \( i \) components of \( s \)

\( \bar{x} = x^{(0)} + y_1v^{(1)} + y_2v^{(2)} + \ldots + y_iv^{(i)} \)

\( s^{(i+1)} = \|b - Ax\|_2 \)

if \( \bar{x} \) is an accurate enough approximation then quit

else \( x^{(0)} = \bar{x} \)

Figure B.2. The Preconditioned Generalized Minimum Residual (GMRES) Algorithm, reprinted from [6].

that the CGS has approximately twice the convergence rate of the BiCG. Alternatively, If the BiCG has irregular convergence, this algorithm has highly irregular convergence. In fact, when the initial guess is very close to the actual solution, the CGS is prone to diverge. \( A^T \) is
Figure B.3. The Preconditioned Biconjugate Gradient Algorithm, reprinted from [6].

never needed in the calculation of the CGS. The algorithm used for the CGS is shown in FIG. B.4 for reference.

B.2.3 The Biconjugate Gradient Stabilized Algorithm

The Biconjugate Gradient Stabilized method (BiCGStab) applies elements of the Conjugate Gradient Squared (CGS) and Generalized Minimum Residuals (GMRES) Algorithms. BiCGStab applies a similar approach as the Conjugate Gradient Squared algorithm [122] to achieve comparable convergence with increased stability. Where the CGS solves for $P_i^2(A)r^{(0)}$ the BiCGStab solves $Q_i(A)P_i(A)r^{(0)}$, where $Q_i(A)$ is an $ith$ degree polynomial describing the steepest descent update. While the CGS can be thought of as a method where the BiCG contraction operator is applied twice, BiCGStab can be thought of...
Compute \( r^{(0)} = b - Ax^{(0)} \) for some initial guess \( x^{(0)} \)

Choose \( \tilde{r} \) (for example, \( \tilde{r} = r^{(0)} \))

for \( i = 1, 2, \ldots \)

\[ \rho_{i-1} = \tilde{r}^T r^{(i-1)} \]

if \( \rho_{i-1} = 0 \) method fails

if \( i = 1 \)

\[ u^{(1)} = r^{(0)} \]

\[ p^{(1)} = u^{(1)} \]

else

\[ \beta_{i-1} = \rho_{i-1} / \rho_{i-2} \]

\[ u^{(i)} = r^{(i-1)} + \beta_{i-1} q^{(i-1)} \]

\[ p^{(i)} = u^{(i)} + \beta_{i-1} (q^{(i-1)} + \beta_{i-1} p^{(i-1)}) \]

endif

solve \( M\hat{p} = p^{(i)} \)

\( \hat{v} = A\hat{p} \)

\[ \alpha_i = \rho_{i-1} / \tilde{r}^T \hat{v} \]

\[ q^{(i)} = u^{(i)} - \alpha_i \hat{v} \]

solve \( M\hat{u} = u^{(i)} + q^{(i)} \)

\[ x^{(i)} = x^{(i-1)} + \alpha_i \hat{u} \]

\[ q = A\hat{u} \]

\[ r^{(i)} = r^{(i-1)} - \alpha_i \hat{q} \]

check convergence; continue if necessary

end

Figure B.4. The Preconditioned Conjugate Gradient Squared Algorithm, reprinted from [6].

as a method applying the product of a BiCG contraction operator and a GMRES contraction operator. The benefit is a fast and stable convergence. The algorithm is shown in FIG. B.5 for reference.

The greatest problem with BiCGStab is that the algorithm is vulnerable to the weaknesses of both the BiCG and the GMRES, i.e. if either would fail, BiCGStab would fail. In these cases there are alternative methods including BiCGStab2 [49] and Bi-CGSTab(L) [112]. Bi-CGStab was first introduced by Henk A. Van Der Vorst in 1991. On the authors website (http://www.math.uu.nl/people/vorst/) it is noted that the Bi-CGSTAB paper was the most cited article in the field of mathematics in the 1990s. The
Compute $r^{(0)} = b - Ax^{(0)}$ for some initial guess $x^{(0)}$.
Choose $\tilde{r}$ (for example, $\tilde{r} = r^{(0)}$)
for $i = 1, 2, \ldots$
\begin{itemize}
  \item $\rho_{i-1} = \tilde{r}^T r^{(i-1)}$
  \item if $\rho_{i-1} = 0$ method fails
  \item if $i = 1$
    \begin{itemize}
      \item $p^{(i)} = r^{(i-1)}$
    \end{itemize}
  \item else
    \begin{itemize}
      \item $\beta_{i-1} = (\rho_{i-1}/\rho_{i-2})(\alpha_{i-1}/\omega_{i-1})$
      \item $p^{(i)} = r^{(i-1)} + \beta_{i-1}(p^{(i-1)} - \omega_{i-1}t^{(i-1)})$
    \end{itemize}
\end{itemize}
solve $M\tilde{p} = p^{(i)}$
$v^{(i)} = \tilde{p}$
$\alpha_i = \rho_{i-1}/\tilde{r}^T v^{(i)}$
$s = r^{(i-1)} - \alpha_i v^{(i)}$
check norm of $s$; if small enough: set $x^{(i)} = x^{(i-1)} + \alpha_i \tilde{p}$ and stop
solve $M s = s$
$t = A \delta$
$\omega_i = t^T s / t^T t$
$x^{(i)} = x^{(i-1)} + \alpha_i \tilde{p} + \omega_i \delta$
$r^{(i)} = s - \omega_i t$
check convergence; continue if necessary
\end{itemize}
for continuation it is necessary that $\omega_i \neq 0$

Figure B.5. The Preconditioned Biconjugate Gradient Stabilized (BiCGStab) Algorithm, reprinted from [6].

website also offers FORTRAN 77 code for the Bi-CGStab(L) method, intended for linear systems involving unsymmetric matrices with complex spectrum.

### B.3 Newton’s Method for Nonlinear Systems

Newton’s Method of root finding is well known as
\begin{equation}
x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)},
\end{equation}
where $f(x)$ is a nonlinear function, and the superscript $k$ indicates a particular iteration. In order to use it, one must be able to explicitly solve for the derivative of $f(x)$. When this can be done, the method has been shown to be quadratically convergent [19]. This system is made simple by the fact that $x$ exists in only a single dimension.

When the function being studied exists in a space larger than a single dimension, Newton’s Method can still be applied. The matrix-vector form of the method is often referred to as the Nonlinear Newton’s Method, which is written
\begin{equation}
x^{k+1} = x^k - [J(x^k)^{-1}] F(x^k),
\end{equation}
where $J(x)$ is the Jacobian matrix of $f(x)$. This formulation is useful in optimization problems where the gradient of the function is known.
where the function \( F(x^k) \) is operating on \( x^k \) which is a vector, and \( J(x^k) \) is the Jacobian. Solving this iteration is made difficult because the jacobian must not only be found, but additionally it must be inverted. The requirement that the jacobian be non-singular can be problematic. The method is generally considered to be quadratically convergent.
APPENDIX C
MODE DECOMPOSITION OF SPATIOTEMPORAL PATTERNS
Mode Decomposition of Spatiotemporal Patterns

Pattern formation governed by complex spatio-temporal dynamics has been studied in many applications, as described in Section 2.1. The qualitative behavior of any pattern-forming system can be studied through a better understood system which has similar symmetry and dynamical properties. In the case of cellular pattern forming systems which involve a quickly moving activator and abundant inhibitor, the Kuramoto-Sivashinsky equation [71, 107] is such a model. Motivated by the new numerical DAF-based scheme that we developed in the previous chapter we explore in this work the formation and evolution of cellular spatiotemporal patterns in $O(2)$ symmetric systems through the Kuramoto-Sivashinsky equation

$$\frac{\partial u}{\partial t} = \eta_1 u - (1 + \nabla^2)^2 u - \eta_2 (\nabla u)^2 - \eta_3 u^3,$$

where $u = u(x; t)$ represents the perturbation of a planar flame front in the direction of propagation, $\eta_1$ measures the strength of the perturbation front, $\eta_2$ is a parameter associated with growth in the direction normal to the burner, and $\eta_3 u^3$ is a term that was added to help stabilize the numerical integration. We choose this model because it is one of the most accurate and well studied examples of the thermo-diffusive instability, and because in previous work [126] it was shown that numerical simulations of the model can capture qualitative features of cellular flames in extended domains. In order to conduct simulations that are relevant to the experiments, i.e., simulations that preserve the $O(2)$ symmetry of the burner, we integrate (C.1) in a circular domain of radius $R$ through polar coordinates $x = (r; \theta)$ and Dirichlet boundary conditions $u(x; t) = 0$ outside of this domain.

In this chapter we review the basic techniques involved in the mode decomposition of spatiotemporal patterns. Section C.1 introduces the Proper Orthogonal Decomposition (POD) that provides for the reduction of a pattern into coherent structures. Additionally, interplay of the energies of the structures describe the exchange of dominance occurring in
the specific pattern. The use of the POD represents an implementation of the Method of Snapshots as discussed in Section C.2.

C.1 Properties of the Proper Orthogonal Decomposition

When analyzing a system for which there is no formal model, a mathematician is likely to adopt a theoretically based model that is optimal in some sense. A good choice is the Proper Orthogonal Decomposition (POD), also known as the Principal Components Analysis (PCA), Singular Value Decomposition (SVD), Singular Systems Analysis, and Karhunen-Loève analysis (KL) [91, 94, 90]. The POD is optimal in the sense that it is able to capture the dominant components of a system using the fewest number of “modes” possible.

In this section we provide a self-contained review of basic definitions and properties of the Proper Orthogonal Decomposition (POD) technique relevant to this work and discuss how the method can be applied to computer simulations in order to separate spatial and temporal behavior. The POD is a well-known technique for determining an optimal basis for the reconstruction of a data set [66, 73]. It has been used in various disciplines that include fluid mechanics [10, 89, 76], identification and control in chemical engineering [47], oceanography [97], image processing [96], and meteorology [75].

Since the kernel is Hermitian, \( R(x, y) = R^*(y, x) \), according to the Riesz Theorem [100], it admits a diagonal decomposition of the form

\[
R(x, y) = \sum_{k=1}^{N} \lambda_k \Phi_k(x) \Phi_k^*(y).
\]  \(\text{ (C.2)}\)

This fact is particularly useful when finding the POD modes analytically. They can be read off of the diagonal decomposition (C.2). Then the temporal coefficients, \( a_k(t_i) \), are calculated by projecting the data set on each of the eigenfunctions

\[
a_k(t_i) = (u(x, t_i), \Phi_k(x)).
\]  \(\text{ (C.3)}\)

It can be shown that both temporal coefficients and eigenfunctions are uncorrelated in time and space, respectively [102, 103, 104]. In addition, the POD modes \( \Phi_k(x) \) and the
corresponding temporal coefficients, \(a_k(t_i)\), satisfy the following orthogonality properties

\[
\begin{align*}
(i) \quad \Phi_j^*(x)\Phi_k(x) &= \delta_{jk}, \\
(ii) \quad \langle a_j(t_i)a_k^*(t_i) \rangle &= \delta_{jk}\lambda_j,
\end{align*}
\]  
\[(C.4)\]  
\[(C.5)\]

where \(\delta_{jk}\) represents the Kronecker delta function. Property (ii) is obtained when the terms in the diagonal decomposition (C.2) are compared with the expression

\[R(x, y) = \sum_{k=1}^{N} \langle a_j(t_i)a_k^*(t_i) \rangle \Phi_k(x)\Phi_k^*(y).\]

The nonnegative and self-adjoint properties of \(R(x, y)\) imply that all eigenvalues are nonnegative and can be ordered accordingly:

\[\lambda_1 \geq \lambda_2 \ldots \geq \ldots \geq 0.\]

Statistically speaking, \(\lambda_k\) represents the variance of the data set in the direction of the corresponding POD mode, \(\Phi_k(x)\). In physical terms, if \(u\) represents a component of a velocity field, then \(\lambda_k\) measures the amount of kinetic energy captured by the respective POD mode, \(\Phi_k(x)\). In this sense, the energy measures the contribution of each mode to the overall dynamics.

The total energy captured in a proper orthogonal decomposition of a numerical or experimental data set is defined as the sum of all eigenvalues

\[E = \sum_{k=1}^{M} \lambda_k.\]  
\[(C.6)\]

The relative energy captured by the \(k\)th mode, \(E_k\), is defined by

\[E_k = \frac{\lambda_k}{\sum_{j=1}^{M} \lambda_j}.\]  
\[(C.7)\]

Note that the cumulative sum of relative energies, \(\sum E_k\), approaches one as the number of modes in the reconstruction increases to \(M\).

Let us consider a sequence of numerical and/or experimental observations represented by scalar functions \(u(x, t_i), i = 1 \ldots M\). Without loss of generality, the time-average of the sequence, defined by

\[\bar{u}(x) = \langle u(x, t_i) \rangle = \frac{1}{M} \sum_{i=1}^{M} u(x, t_i),\]  
\[(C.8)\]
is assumed to be zero. The Proper Orthogonal Decomposition extracts time-independent orthonormal basis functions, $\Phi_k(x)$, and time-dependent orthonormal amplitude coefficients, $a_k(t_i)$, such that the reconstruction

$$u(x, t_i) = \sum_{k=1}^{M} a_k(t_i) \Phi_k(x), \quad i = 1, \ldots, M,$$

is optimal in the sense that the average least squares truncation error

$$\varepsilon_m = \left\langle \left\| u(x, t_i) - \sum_{k=1}^{m} a_k(t_i) \Phi_k(x) \right\|^2 \right\rangle,$$

is minimized for any given number $m \leq M$ of basis functions over all possible sets of orthogonal functions. Here $\| \cdot \|$ is the $L^2$-norm, $\| f \|^2 = (f, f)$, where $(\cdot, \cdot)$ denotes the standard Euclidean inner product; $\langle \cdot \rangle$ denotes an average operation, usually over time; and the functions $\Phi_k(x)$ are called empirical eigenfunctions, coherent structures, or POD modes.

In practice the state of a numerical model is only available at discrete spatial grid points, so that the observations that form the data set are vectors rather than continuous functions. In other words, $D = (x_1, x_2, \ldots, x_N)$, where $x_j$ is the $j$-th grid point and $u(x, t_i)$ is the vector $u_i = [u(x_1, t_i), u(x_2, t_i), \ldots, u(x_N, t_i)]^T$. The data set can be obtained from numerical simulation, experimental investigation or a combination of the numerical and experimental results. More importantly, it can be shown that the eigenfunctions $\Phi_k$ are the eigenvectors of the the tensor product matrix

$$R(x, y) = \frac{1}{M} \sum_{i=1}^{M} u_i u_i^T.$$

The shifting of the coherent structures over time describe the dynamics of the system, and represent a decomposition of the spatiotemporal pattern of the system [94]. Once this information is obtained, we can compare the relationships between the modes of the system that correspond to a steady state. By analyzing the amplitude changes over time, we can understand how these structures correlate to each other. The relative phase $\Theta_{mn}$ describes the angular displacement of the amplitudes of modes $\Phi_m$ and $\Phi_n$ in relation
to each other. It is calculated as follows:

\[ \Theta_{mn}(t_i) = \tan^{-1} \left( \frac{a_n(t_i)}{a_m(t_i)} \right). \] (C.12)

When the relative phase line is linear, we know that the modes are changing in amplitude in linear relation to each other. This is common in flame systems when the system is changing position uniformly over time, for instance if the system is experiencing a rigid rotation. When the flames are changing shape as well as position over time, it is likely that the amplitudes of the modes will not evolve in linear relation to each other. In these cases the relative phase plot will display an oscillatory line. This is the trademark of a modulated rotation, and has been described by Antonio Palacios [90].

Another sort of plot used to describe the relationships is the phase plane. In these plots the amplitude for one mode is plotted against the amplitude for another. Once again, the modes whose amplitudes exhibit a regular, circular plot are oscillating in concert. These occur in systems that are changing uniformly over time. Modulated rotations often result in plots that appear as thicker circles or more complex shapes. Examples of phase plane projections are shown later in FIG. 4.6 and FIG. 4.9.

C.2 Computational Implementation: Method of Snapshots

A popular technique for finding the eigenvectors of (C.11) is the method of snapshots developed by Sirovich [102, 104]. It was introduced as an efficient method when the resolution of the spatial domain (N) is higher than the number of observations (M). The method of snapshots is based on the fact that the data vectors, \( u_i \), and the eigenvectors \( \Phi_k \), span the same linear space [89]. This implies that the eigenvectors can be written as a linear combination of the data vectors

\[ \Phi_k = \sum_{i=1}^{M} v_i^k u_i, \ k = 1..M. \] (C.13)

After substitution in the eigenvalue problem, \( R(x; y) \Phi(y) = \lambda \Phi(x) \), the coefficients \( v_i^k \) are obtained from the solution of

\[ Cv = \lambda v, \] (C.14)
where $v_k = (v_k^1, \ldots, v_k^M)$ is the kth eigenvector of (C.14), and $C$ is a symmetric $M \times M$ matrix defined by $[c_{ij}] = \frac{1}{M}(u_i, u_j)$. Here $(\cdot, \cdot)$ denotes the standard vector inner product, $(u_i, u_j) = u(x_1, t_i) u(x_1, t_j) + \ldots + u(x_N, t_i) u(x_N, t_j)$. In this way the eigenvectors of the $N \times N$ matrix $R$ (C.11) can be found by computing the eigenvectors of an $M \times M$ matrix $C$ (C.14), a preferable task if $N \gg M$.

In this analysis, thousands of frames from the steady state pattern were used to find a basis set of eigenfunctions of a certain steady state, via the Proper Orthogonal Decomposition. This type of analysis is an implementation of the method of snapshots.