INTEGRATING THE KURAMOTO-SIVASHINSKY EQUATION: A SIMULATION OF THE HOPPING STATE

A Thesis
Presented to the
Faculty of
San Diego State University

In Partial Fulfillment
of the Requirements for the Degree
Master of Science
in
Computational Science

by
Scott Arthur Gasner
Fall 2004
THE UNDERSIGNED FACULTY COMMITTEE APPROVES
THE THESIS OF SCOTT ARTHUR GASNER:

Peter Blomgren, Chair
Department of Mathematics and Statistics

Antonio Palacios
Department of Mathematics and Statistics

Subrata Bhattacharjee
Department of Mechanical Engineering

SAN DIEGO STATE UNIVERSITY
Fall 2004
DEDICATION

Thanks to my wife Kelly,
for without her I would not be here.

Thanks to my father Larry,
my mother Lovice, and my brothers Glenn and Paul,
for their insight and encouragement.

Best wishes to all of my fellow students at
San Diego State University.
ACKNOWLEDGEMENTS

Thanks to the professors and administrators of the San Diego State University Computational Science Research Center and to all of my professors at the San Diego State University Department of Mathematics and Statistics. Special thanks to Prof. Peter Blomgren and Prof. Antonio Palacios who have been at the same time helpful and inspirational in the research of the thesis. Special Thanks to Dr. Jose Castillo for his continued support.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>ACKNOWLEDGEMENTS</th>
<th>iv</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIST OF FIGURES</td>
<td>viii</td>
</tr>
<tr>
<td>CHAPTER</td>
<td></td>
</tr>
<tr>
<td>1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>2. BACKGROUND</td>
<td>3</td>
</tr>
<tr>
<td>2.1 The Kuramoto-Sivashinsky Equation</td>
<td>4</td>
</tr>
<tr>
<td>2.1.1 Cellular Flame Fronts</td>
<td>6</td>
</tr>
<tr>
<td>2.1.2 Derivation of the Kuramoto-Sivashinsky Equation</td>
<td>7</td>
</tr>
<tr>
<td>2.2 Physical Experimentation</td>
<td>10</td>
</tr>
<tr>
<td>3. NONLINEAR NUMERICAL INTEGRATION</td>
<td>13</td>
</tr>
<tr>
<td>3.1 Construction of the Integration Scheme</td>
<td>13</td>
</tr>
<tr>
<td>3.1.1 The Interpolating Distributed Approximating Functionals</td>
<td>15</td>
</tr>
<tr>
<td>3.2 Time Integration of the Kuramoto-Sivashinsky Equation</td>
<td>16</td>
</tr>
<tr>
<td>3.2.1 The Zhang, et. al. Approach</td>
<td>17</td>
</tr>
<tr>
<td>3.2.2 The Crank-Nicolson Based Approach</td>
<td>18</td>
</tr>
<tr>
<td>4. MODE DECOMPOSITION OF SPATIOTEMPORAL PATTERNS</td>
<td>21</td>
</tr>
<tr>
<td>4.1 Properties of the Proper Orthogonal Decomposition</td>
<td>21</td>
</tr>
<tr>
<td>4.2 Computational Implementation: Method of Snapshots</td>
<td>25</td>
</tr>
<tr>
<td>5. NUMERICAL EXPLORATION</td>
<td>26</td>
</tr>
<tr>
<td>CHAPTER</td>
<td>PAGE</td>
</tr>
<tr>
<td>---------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>5.1 Stability Analysis</td>
<td>26</td>
</tr>
<tr>
<td>5.2 Bifurcation Analysis</td>
<td>27</td>
</tr>
<tr>
<td>6. CONCLUSION AND FURTHER RESEARCH</td>
<td>37</td>
</tr>
<tr>
<td>BIBLIOGRAPHY</td>
<td>38</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>43</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

FIGURE PAGE

2.1 The bunsen flame separation experiment by Smithells and Ingle in 1891 [64] 3

2.2 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. 12

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. \( dr = \frac{R}{32.5} \) and \( d\phi = \frac{2\pi}{64} \). 14

5.1 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 \( \Psi_{33} \). 27

5.2 Marginal stability curves outline the stability domains where the trivial solution \( u_0 = 0 \) (representing a uniform flame front) bifurcates to Fourier–Bessel modes \( \Psi_{nm} \). 28

5.3 Ten sequential time (top index) snapshots of a dynamic state of three cells rotating counterclockwise, with small modulations, found in simulations of (3.1). Parameter values are: \( \epsilon = 0.32, \eta_1 = 1.0, \eta_2 = 0.013, \) and \( R = 7.36 \). 29

5.4 POD decomposition of a single ring state with three cells rotating uniformly and counter-clockwise. 29

5.5 (left) Phase-space projections and (b) phase-angles produced by the time coefficients of the POD decomposition of the rotating pattern shown in figure 5.3 suggest that the pattern rotates uniformly. 31

5.6 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: \( \epsilon = 0.32, \eta_1 = 1.0, \eta_2 = 0.013, \) and \( R = 7.7475 \). 32

5.7 POD decomposition of hopping motion from a three-cells patterns found in simulations of (3.1). 33

5.8 (Top) Phase-space projections produced by the time coefficients of the POD decomposition of the rotating pattern shown in figure 5.6; (bottom) Associated relative phase angles. 35

5.9 Reconstruction of the hopping state with \( M = 9 \) modes. 35
5.10 Reconstruction of the hopping state with $M = 9$ modes, excluding modes $\Phi_3$, $\Phi_4$, and $\Phi_5$. 

36
CHAPTER 1

INTRODUCTION

Premixed gases burn irregularly, which can lead to cellular flame patterns [16] formed through a mechanism that resembles that of reaction-diffusion systems described first by Turing [66]. When the gases are confined to circular domains, the cells generically 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 [19]. An individual pattern, either stationary or nonstationary, is selected based on control parameters such as type of fuel, pressure, flow rate and fuel-to-oxidizer ratio. In previous work [48], the behavior of certain dynamic patterns, called hopping states were analyzed [16, 18]. It was found that individual cells sequentially made abrupt changes in their angular positions while they kept rotating in a ring structure. The study found isolated rings of hopping states as well as concentric rings of cells in which the outer ring remains stationary while the inner ring exhibited hopping motion. The analysis was based solely on experimental data and the use of the Proper Orthogonal Decomposition (POD), which is also known as the Singular Value Decomposition (SVD) [48]. A comparative analysis against computer-simulated hopping states was precluded by the lack of a reliable model of the combustion of premixed gases that can produce solutions with truly two-dimensional features similar to those observed in experiments [8]. There have been, however, reports of similar states, described as Pushme-Pullyou, found in a quasi-one-dimensional thermo-diffusive model [3].

This thesis reports a new numerical integration scheme through which we have observed for the first time a truly 2D hopping state. The state was found in simulations of the Kuramoto-Sivashinsky (KS) model [36, 60], which is considered to be one of the simplest models of thermodiffusive instability and one that can produce solutions that closely resemble experimental states, including stationary and dynamic patterns. The actual hopping state is
a single-ring state made up of three cells and it was 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. In this paper, we discuss these similarities and differences in more detail.

The paper is organized as follows. In Chapter 2 we introduce the Kuramoto-Sivanshinsky equation and discuss the history of its derivation. Then the combustion experiment that is the physical basis of this study is described. In Chapter 3 we describe the Numerical Integration Scheme that was developed for this study. The Crank-Nicolson Method is described along with the implementations of other numerical methods. In Chapter 4 we present the POD based mode decomposition approach to describing the patterns formed by the system and review the basic principles and properties of the Proper Orthogonal Decomposition relevant to this work. Chapter 5 describes one particular method for searching for hopping states in parameter space. We report the location in parameter space in which the hopping state has be found, and describe the observed spatio-temporal dynamics. Then we compare the newly found state with another similar state through bifurcation analysis. We report a difference between the numerically simulated hopping state and the experimentally observed hopping state, and propose an explanation. Chapter 6 concludes the work and presents the opportunities for further research.
CHAPTER 2

BACKGROUND

Smithells and Ingle reported their observations of bunsen burner flames in 1892. They were able to discern two conical flame fronts, one inside of the other. While experimenting with benzene, they noted that when the gas 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. They were the first to report a cellular flame pattern, 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. [64]”

Figure 2.1: The bunsen flame separation experiment by Smithells and Ingle in 1891 [64]

In 1977 Gregory I. Sivashinsky determined an equation for a “laminar flame front” [60]. Another scientist, Yoshiki Kuramoto, developed the same equation at the same time while modeling diffusion-induced chaos [36] in a study of the Belousov-Zabotinskii reaction in three dimensions [29]. Their joint discovery is known as the Kuramoto-Sivashinsky Equation.

Sivashinsky published papers concerning flame dynamics. A sample of topics include: the
Flame dynamics exhibit diffusion-induced chaos. 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. The study of pattern formation is the study of being able to describe the “type” of outcome for a physical experiment with a large degree of certainty, even though the exact solution cannot be predicted. Thus it became a significant physiological phenomenon to chaos theory mathematicians. Studies have investigated the bifurcation phenomena in burner-stabilized premixed flames [40]; conductive interactions of wrinkled flames with cold flat burners [32]; stability of the porous plug burner flame [7]; viscoelastic behavior of cellular solutions to the Kuramoto-Sivashinsky model [14]; approximate inertial manifolds for the Kuramoto-Sivashinsky equation [31]; bifurcations and pattern formation in the regularized Kuramoto-Sivashinsky equation [6]; nonlinear dynamics of cellular flames [4]; and the transition to spatiotemporal chaos in the damped Kuramoto-Sivashinsky equation [12] among many other topics. While much work has been done, few have numerically simulated a two dimensional flame front, and none have numerically simulated the hopping state.

2.1 The Kuramoto - Sivashinsky Equation

When a premixed gas is burning, the rate of the reaction (W) is proportional to the temperature. 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).

\[ W \sim \exp\left(-\frac{E}{RT}\right). \]  \hfill (2.1)

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 transitional 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

\[ U_u = \sqrt{\frac{2D_{th}}{T_b - T_u} \int_{T_u}^{T_b} W(C, T) \, dT}. \]  \hfill (2.2)

\( T_u \) 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 \( \ell_{th} \approx 0.05cm \) \[57\].

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 [67]. However, for combustion over wide apertures the flame commonly breaks up into separate cells $\sim 1$ cm to $10$ cm in size. Cellular flames also appeared to have a regular underlying two or three dimensional structure despite the constant subdivision and recombination of the cells [57].

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, taking a three dimensional reaction region to a two dimensional reactive front. Due to Arrhenius kinetics this would actually be the case for a combustion requiring an infinitely large activation energy [39]. Thus we are able to simulate the three dimensional flame with a two dimensional surface.

### 2.1.1 Cellular Flame Fronts

In understanding the dynamics of flames, Sivashinsky tried to qualitatively understand the forces driving the shape of the flame front. He found that the conduction of heat has a stabilizing effect on flames [59]. 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 [59].

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 [59].

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 [50].

The hydrodynamics of the underlying mixture will directly effect the behavior of the flame front, and can produce corrugated and cellular flame front structures [13]. 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 completely described without introducing the effects of the hydrodynamics of the mixture. 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. This can be done if we also assume that the density of the gas is constant. Then the thermal perturbations cannot be transformed into hydrodynamic perturbations, and the problem of hydrodynamics is separated completely from that of combustion proper [59].

2.1.2 Derivation of the Kuramoto-Sivashinsky Equation

Now that we have described the assumptions to our model, we derive the nonlinear model for thermal-diffusive flame instability. A perturbation analysis of laminar flames lead to the understanding that a plane flame front may be unstable to long-wave disturbances. The effect of a long-wave disturbance is described by the dispersion relation [1]:

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

(2.3)

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 \( F \sim \exp(\sigma t + i k \cdot x) \) [57] 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 [59] that although a plane flame front may be unstable to long-wave perturbations, it always stable with regards to short-wave perturbations. Therefore a nonlinear term is needed to describe this stability to short-wave disturbances. The following was derived for systems where $\text{Le} \cong \text{Le}_c$:

$$\sigma = D_{th}\frac{1}{2}\beta(1 - \text{Le}) - 1]k^2 - 4D_{th}\ell_{th}^2k^4.$$  \hspace{1cm} (2.4)

Thus a system is stable when the diffusivity of the limiting reactant is less than a critical value ($\text{Le} > \text{Le}_c = 1 - \frac{2}{\beta}$). When $\text{Le} < \text{Le}_c$ 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 [57].

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:

$$F_t + D_{th}\frac{1}{2}\beta(1 - \text{Le}) - 1]\nabla^2 F + 4D_{th}\ell_{th}^2\nabla^4 F = 0.$$ \hspace{1cm} (2.5)

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. If 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:

$$F_t = U_b(1 - \sqrt{1 + (\nabla F)^2}).$$ \hspace{1cm} (2.6)

When a system that is near the stability threshold $\text{Le} \cong \text{Le}_c$, the gradient of the flame front should be small, and therefore $(\nabla F)^2 \ll 1$. Hence

$$F_t + \frac{1}{2}U_b(\nabla F)^2 = 0.$$ \hspace{1cm} (2.7)

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:

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

(2.8)

For behavioral study this equation may be stated in a non dimensional way:

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

(2.9)

Sivashinsky recognized that this model had the ability to describe the chaotic motion of cells, and said “Quite likely the model also describes polyhedral, rotating bunsen flames and the apparently similar phenomenon of traveling waves that sometimes appear in place of chaotically recombining cells.” [57]

Acknowledging 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, \( g (1 - \epsilon) / 2 U_b \) where \( \epsilon = \rho_b / \rho_u \), was added to the equation to account for this force. The equation was then revised from (2.9) to the following:

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

(2.10)

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:

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

(2.11)

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 [10].
2.2 Physical Experimentation

Combustion Experiments were conducted by M. Gorman at the University of Houston [19]. A mixture of isobutane 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 1/30sec 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. O(2) symmetry implies the flame pattern is invariant under any rotation and under reflection in a two dimensional euclidean space. As the system dynamics are altered through the parameters, the system bifurcates into more complex patterns through a sequence of symmetry breaking bifurcations.

Of particular interest to this thesis are a special type of nonuniformly traveling wave patterns, 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. Figure 2.2 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 [50]. For instance, hopping cells do not rotate rigidly. 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. Note that the characteristics of this nonuniform motion are also very different from the synchronous modulated dynamics of Modulated Travelling Waves (MTWs) [3].
Figure 2.2: 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.
CHAPTER 3

NONLINEAR NUMERICAL INTEGRATION

The numerical scheme discussed in this thesis is an extension of [68] which proposes a scheme for the time-integration of the Kuramoto-Sivanshinsky equation. The scheme proposed is second order in time. Further, the new scheme, in which the time-integration is based on the Crank-Nicolson method [9], is unconditionally A-stable, thus producing finite solutions in all cases where the exact solution of the underlying equation produces finite solutions.

This stable scheme allows for the simulation of many thousand frames of the Kuramoto-Sivanshinsky (KS) equation. For this study we used the following form of the KS:

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

(3.1)

which is described in detail in chapter 4. The KS (3.1) can be written in polar coordinates as

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

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

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

(3.2)

The A-stable Crank-Nicolson scheme is coupled with an iterative Newton solver in order to integrate the nonlinear terms in time. 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.

3.1 Construction of the Integration Scheme

Numerical investigation of cellular flames in a circular burner using the Kuramoto-Sivanshinsky equation (3.1) has been elusive due to the singularity that arises in the biharmonic operator, \( \nabla^4 = (\partial_{rr} + 2\frac{1}{r}\partial_r + \frac{1}{r^2}\partial\phi\phi)^2 \), near the origin of the polar grid. Even
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 $d\phi = \frac{2\pi}{64}$.

though the singularity can be avoided by partitioning each diameter into an even number of equally spaced lattice points (see Figure 3.1), the presence of small denominators, i.e. $\frac{1}{r^4} \partial_{\phi\phi\phi\phi}$, at points close to the origin make the resulting system quite ill-conditioned and extremely sensitive to errors in the spatial derivatives. The algorithm presented in [68] utilizes Distributed Approximating Functionals [25] and aims at approximating the flame front $u(r, \phi, t)$ and its spatial derivatives to high accuracy on and off the grid points.

Even though great care was taken in [68] to develop an algorithm which captures the spatial derivative to high accuracy, it turns out that the algorithm is not well suited for long-time integration, especially of complex patterns, due to an instability caused by the treatment of the temporal derivative.
In section 3.1.1 we review distributed approximating functionals. Then, in section 3.2.1 we describe the weakness in the temporal approximation scheme used in [68]. In section 3.2.2 we propose an alternative treatment of the temporal derivative.

### 3.1.1 The Interpolating Distributed Approximating Functionals

The Interpolating Distributed Approximating Functionals (DAFs) have been extensively described [24, 35, 68, 25, 26, 28] and successfully applied to a wide range of applications, e.g. atom-atom potentials [15], ro-vibrational states of H$_3^+$ [30], path-integrals for quantal many-body dynamics [34], and the Fokker-Planck equation [69] 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:

\[
f(x) = \int_{-\infty}^{\infty} \delta(x - x') f(x') dx' \tag{3.3}
\]

\[
f^{\ell}(x) = \int_{-\infty}^{\infty} \delta^{(\ell)}(x - x') f(x') dx', \tag{3.4}
\]

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

\[
I(x - x') = \frac{1}{\sigma} \exp(-z^2) \sum_{n=0}^{M/2} \left(-\frac{1}{4}\right)^n \frac{1}{\sqrt{2\pi n!}} H_{2n}(z), \tag{3.5}
\]

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

\[
f(x) \approx f_{DAF}(x) = \int_{-\infty}^{\infty} I(x - x') f(x') dx'. \tag{3.6}
\]
The DAF also allows for derivatives of the approximated function to be evaluated as

\[ f^{(\ell)}(x) \approx f_{DAF}^{(\ell)}(x) = \int_{-\infty}^{\infty} I^{(\ell)}(x - x') f(x') dx', \tag{3.7} \]

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

\[ I^{(\ell)}(x - x') = \frac{2^{-\ell/2}}{\sigma^{\ell + 1}} \exp(-z^2) \sum_{n=0}^{M/2} \left(-\frac{1}{4}\right)^n (-1)^\ell \frac{1}{\sqrt{2\pi n!}} H_{2n+1}(z). \tag{3.8} \]

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

\[ f(x) \approx f_{DAF}(x) = \Delta \sum_j I(x - x_j) f(x_j) \tag{3.9} \]

\[ f^{(\ell)}(x) \approx f_{DAF}^{(\ell)}(x) = \Delta \sum_j I^{(\ell)}(x - x_j) f(x_j), \tag{3.10} \]

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 (Figure 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 in fact 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. [27] 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 Time Integration of the Kuramoto-Sivashinsky Equation

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.

\[
    F_{\text{lin}}(\vec{x}, t, u(t)) = -u_{rrrr} - \frac{1}{r^4} u_{\phi\phi\phi\phi} - \frac{2}{r^2} u_{rr\phi\phi} - \frac{2}{r} u_{rrr} + \frac{2}{r^3} u_{r\phi\phi} - \left[ 2 - \frac{1}{r^2} \right] u_{rr} - \left[ \frac{4}{r^4} + \frac{2}{r^2} \right] u_{\phi\phi} - \left[ \frac{1}{r^3} + \frac{2}{r} \right] u_r + \epsilon u.
\]

We now focus

\[
    F_{\text{nl}}(\vec{x}, t, u(t)) = -\eta_1 \left[ u_r^2 + \frac{1}{r^2} u_\phi^2 \right] - \eta_2 u^3.
\]

We note that with the DAF-representation every spatial derivative can be expressed as a sum over the domain, with appropriate weights, e.g.

\[
    u_{rr}(r, \phi) = \sum_{r_i=1, \phi_i=1}^{N_r, N_\phi} w_{rr}^\text{DAF} \cdot (r_i - r, \phi_i - \phi) u(r_i, \phi_i),
\]

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 once and for all. We now focus
our attention to the treatment of the non-linear term $F_{nl}(\vec{x}, t, u(t))$.

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

In [68] the proposed DAF-based time-integration scheme for the Kuramoto-Sivanshinsky model is expressed in the form

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

(3.13)

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, $F_{nl}(\vec{x}, t, u(t))$ 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)

$$\left[\frac{u_x(t + h) + u_x(t)}{2}\right]^2 = \frac{1}{4} \left[u_x(t + h)^2 + 2u_x(t + h)u_x(t) + u_x(t)^2\right], \quad s = \{r, \phi\}.\quad (3.15)$$

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

$$\left[\frac{u(t + h) + u(t)}{2}\right]^3 \approx \frac{-u(t)^3}{2} + \frac{3u(t)^2u(t + h)}{2}\quad (3.16)$$

$$\left[\frac{u_x(t + h) + u_x(t)}{2}\right]^2 \approx u_x(t)u_x(t + h),\quad (3.17)$$

where in (3.17) $s = \{r, \phi\}$. The scheme can be shown to have second and third order error terms. These error terms cannot be easily controlled. In practice 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 within a couple of hundred iterations, even for relatively simple patterns. A very stable scheme was necessary to allow for a tight control on the error allowed at each step.
3.2.2 The Crank-Nicolson Based Approach

We propose a time-integration algorithm based on the Crank-Nicolson [9] scheme. With $F(\bar{x}, t, u(t))$ as before, we write

$$\frac{u(t+h) - u(t)}{h} = \frac{F(x, t, u(t)) + F(x, t + h, u(t + h))}{2}.$$  (3.18)

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 [65], and makes the time-discretization truly second order. Furthermore, by keeping the full non-linearity of $F(\cdot)$, the spatial approximation retains the order of the DAF-approximation.

With the spatial derivatives in (3.18) represented by the DAF-approximations (3.12) we get a non-linear system of equations (3.19)

$$\bar{G}(\bar{u}(\bar{x}, t + h)) = 0,$$  (3.19)

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

$$\bar{u}^{n+1}(\bar{x}, t + h) = \bar{u}^{n}(\bar{x}, t + h) - \left[\delta \bar{G}(\bar{u}^{n}(\bar{x}, t + h))\right]^{-1} \cdot \bar{G}(\bar{u}^{n}(\bar{x}, t + h)),$$  (3.20)

$$\bar{u}^{0}(\bar{x}, t + h) = \bar{u}(\bar{x}, t),$$  (3.21)

where $\delta \bar{G} = \nabla_{\bar{u}} \bar{G}(\bar{u}^{n}(\bar{x}, t + h))$ is the Jacobian. The Newton-iteration is repeated until the residual is reduced sufficiently, e.g.

$$\|\bar{G}(\bar{u}^{n+1}(\bar{x}, t + h))\| \leq \text{tol} \cdot \|\bar{G}(\bar{u}^{0}(\bar{x}, t + h))\|.$$  

In each step of the Newton-iteration we have to solve the linear system

$$\left[\delta \bar{G}(\bar{u}^{n}(\bar{x}, t + h))\right] \delta \bar{u} = \bar{G}(\bar{u}^{n}(\bar{x}, t + h)),$$

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 biconjugate gradient stabilized method (Bi-CGSTAB) [2], where a
good preconditioner can be extracted by noticing that the equations (3.19) decompose in linear and non-linear contributions

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

(3.22)
corresponding directly with the decomposition of $F(\vec{x}, t, u(t)) = F_{\text{lin}}(\vec{x}, t, u(t)) + F_{\text{nl}}(\vec{x}, t, u(t))$ in (3.11). This decomposition is transitive to the Jacobian, and we have

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

(3.23)
where $\delta \vec{G}_{\text{lin}}(\vec{u}(\vec{x}, t+h)) = M$ is constituted from contributions from DAF-derivative coefficients (3.12) and therefore does not depend on $\vec{u}(\vec{x}, t+h)$. $M$, and its $LU$-decomposition can be computed once and serves as the preconditioner for the Bi-CGSTAB($M$) algorithm.
CHAPTER 4

MODE DECOMPOSITION OF SPATIOTEMPORAL PATTERNS

Pattern formation governed by complex spatio-temporal dynamics has been studied in many applications, e.g. chemical systems [44], fluid convection [23], flame-front propagation [19, 16, 18, 17], etc. The qualitative behavior of a pattern-forming system can be studied using simplified models. In the case of cellular flames stabilized on a circular porous plug burner, the Kuramoto-Sivashinsky equation [36, 59, 60] is such a model. Motivated by the new numerical DAF-based scheme that we developed in chapter 3 we explore in this work the formation and evolution of hopping states through the Kuramoto-Sivashinsky equation

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

where $u = u(x; t)$ represents the perturbation of a planar flame front in the direction of propagation, $\epsilon$ measures the strength of the perturbation front, $\eta_1$ is a parameter associated with growth in the direction normal to the burner, and $\eta_2 u^3$ is a term that was added to help stabilize the numerical integration. We choose this model because it is one of the simplest models of the thermo-diffusive instability [36, 60], and because in previous work [68] 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 (3.1) 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. Our aim in this chapter is to describe how we use the numerical simulations to gain insight into the underlying bifurcations that lead to hopping states. We treat the radius of the burner as the distinguished bifurcation parameter, while the other parameters are held fixed.

4.1 Properties of the Proper Orthogonal Decomposition

The process of describing the underlying dynamics of a flame pattern is incumbered by the lack of a formal model. Rather than describing the underlying structures using physics
or engineering methods, the complexity of the flames have left little recourse other than
the purely mathematical. Significant results have been found using the Proper Ortho-
gonal Decomposition (POD), also known as the Principal Components Analysis (PCA), Singu-
lar Value Decomposition (SVD), Singular Systems Analysis, and Karhunen-Loéve analysis
(KL) [47, 50, 46].

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. Readers familiar with the technique can skip this section. The POD is a well-known
 technique for determining an optimal basis for the reconstruction of a data set [33, 37]. It
has been used in various disciplines that include fluid mechanics [5, 45, 38], identification and
control in chemical engineering [21], oceanography [52], and image processing [51].

Since the kernel is Hermitian, \( R(x, y) = R^*(y, x) \), according to the Riesz Theorem [53],
it admits a diagonal decomposition of the form

\[
R(x, y) = \sum_{k=1}^{N} \lambda_k \Phi_k(x) \Phi_k^*(y). \tag{4.2}
\]

This fact is particularly useful when finding the POD modes analytically. They can be read off
of the diagonal decomposition (4.2). Then the temporal coefficients, \( a_k(t_i) \), are calculated
by projecting the data set on each of the eigenfunctions

\[
a_k(t_i) = \langle u(x, t_i), \Phi_k(x) \rangle. \tag{4.3}
\]

It can be shown that both temporal coefficients and eigenfunctions are uncorrelated in time
and space, respectively [45, 54, 55, 56]. In addition, the POD modes \( \Phi_k(x) \) and the corre-
sponding temporal coefficients, \( a_k(t_i) \), satisfy the following orthogonality properties

\[
(i) \quad \Phi_j^*(x) \Phi_k(x) = \delta_{jk}, \tag{4.4}
\]

\[
(ii) \quad \langle a_j(t_i) a_k^*(t_i) \rangle = \delta_{jk} \lambda_j. \tag{4.5}
\]

where \( \delta_{jk} \) represents the Kronecker delta function. Property (ii) is obtained when the
terms in the diagonal decomposition (4.2) are compared with the expression

\[
R(x, y) = \sum_{k=1}^{N} \lambda_k \Phi_k(x) \Phi_k^*(y). \tag{4.2}
\]
\[ \sum_{k=1}^{N} (a_j(t_i) a_k^*(t_i)) \Phi_k(x) \Phi_k^*(y). \]

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

\[ E = \sum_{k=1}^{M} \lambda_k. \]  \hspace{1cm} (4.6)

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

\[ E_k = \frac{\lambda_k}{\sum_{j=1}^{M} \lambda_j}. \]  \hspace{1cm} (4.7)

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

\[ \bar{u}(x) = \langle u(x, t_i) \rangle = \frac{1}{M} \sum_{i=1}^{M} u(x, t_i), \]  \hspace{1cm} (4.8)

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

\[ u(x, t_i) = \sum_{k=1}^{M} a_k(t_i) \Phi_k(x), \quad i = 1, \ldots, M, \]  \hspace{1cm} (4.9)

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

\[ \varepsilon_m = \left\langle \left\| u(x, t_i) - \sum_{k=1}^{m} a_k(t_i) \Phi_k(x) \right\|^2 \right\rangle, \]  \hspace{1cm} (4.10)
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

\[
R(x, y) = \frac{1}{M} \sum_{i=1}^{M} u_i u_i^T. \tag{4.11}
\]

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 [50]. Once this information is obtained, we can compare the relationships between the modes of the system that correspond to a steady state. By analysing 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:

\[
\Theta_{mn}(t_i) = \tan^{-1}\left( -\frac{a_n(t_i)}{a_m(t_i)} \right). \tag{4.12}
\]

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 [46].

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.

The results of these plots for a hopping state are shown after further discussion in Figure 5.8.

### 4.2 Computational Implementation: Method of Snapshots

A popular technique for finding the eigenvectors of (4.11) is the *method of snapshots* developed by Sirovich [54, 56]. 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 [45, 54]. This implies that the eigenvectors can be written as a linear combination of the data vectors

$$\Phi_k = \sum_{i=1}^{M} v^k_i u_i, \quad k = 1..M. \quad (4.13)$$

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

$$Cv = \lambda v, \quad (4.14)$$

where $v_k = (v^k_1, \ldots, v^k_M)$ is the kth eigenvector of (4.14), 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 $R$ (4.11) can be found by computing the eigenvectors of an $M \times M$ matrix $C$ (4.14), 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.
CHAPTER 5

NUMERICAL EXPLORATION

5.1 Stability Analysis

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

\[
w(r, \theta, t) = e^{\lambda t} \Psi_{nm}(r, \theta) + c.c., \tag{5.1}
\]

where \( \Psi_{nm}(r, \theta) = J_n(\alpha_{nm} r / R)e^{in\theta}, \quad (m \geq 0 \text{ and } n > 0) \) 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 Figure 5.1, is a natural choice [49]. Now substituting (5.1) into (3.1) and using the fact that \( \nabla^2 \Psi_{nm} + k^2 \Psi_{nm} = 0 \), and \( \nabla^4 \Psi_{nm} - k^4 \Psi_{nm} = 0 \), where \( k^2 = (\alpha_{nm} / R)^2 \), 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

\[
\varepsilon_{nm}(R) = 1 - 2 \left( \frac{\alpha_{nm}}{R} \right)^2 + \left( \frac{\alpha_{nm}}{R} \right)^4. \tag{5.2}
\]

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
Figure 5.1: 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 $\Psi_{33}$.

5.2 Bifurcation Analysis

The stability analysis lead us to a region in parameter space where the evolution of a single-ring pattern with three cells can be traced. Such region can be found in a neighborhood of the minimum of the marginal stability curve $B_{31}$ shown in Figure 5.2. 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 5.2: Marginal stability curves outline the stability domains where the trivial solution $u_0 = 0$ (representing a uniform flame front) bifurcates to Fourier–Bessel modes $\Psi_{nm}$.

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. Figure 5.3 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.

An ensemble of 2000 consecutive snapshots was generated for the POD analysis. Figure 5.4 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 4.1 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 [11]. 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 5.4: POD decomposition of a single ring state with three cells rotating uniformly and counterclockwise.

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 [50, 49]. 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 Figure 5.3 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 Figure 5.5 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

$$u(x, t) = \tilde{u} + \sum_{k=1}^{M} a_k(t)\Phi_k(x)$$

(5.3)

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 [22, 50] 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 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 [18, 48]. This last assertion is not a big surprise giving the fact that in a POD decomposition of experimental hopping states [48] we found similar modes to those shown in Figure 2.2. In particular, we found $\Phi_1, \Phi_2, \Phi_7, \Phi_8, \Phi_9,$ and $\Phi_{10},$ 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 $\Phi_5$. Interestingly, now the reconstructed dynamics resembles 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 Figure 5.3 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 [16, 18]. Figure 5.6 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 5.6: 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: $\epsilon = 0.32$, $\eta_1 = 1.0$, $\eta_2 = 0.013$, and $R = 7.7475$.](image)

An ensemble of 6000 consecutive snapshots was generated for the POD decomposition. Figure 5.7 shows the time-average, principal modes, and POD energy, in the same format as they appeared in Figure 5.4. 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 Figure 5.7, do not appear in Figure 5.4. Mode \( \Phi_{10} \) in Figure 5.7 corresponds to mode \( \Phi_{11} \) in Figure 5.4, though this mode is not shown in Figure 5.4. Modes \( \Phi_3 \) and \( \Phi_4 \) in Figure 5.7 can be thought 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 Figure 5.7.

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.

Figure 5.7 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. Figure 5.8 shows the phase plane plots for the most energetic modes.

Figure 5.7: POD decomposition of hopping motion from a three-cells patterns found in simulations of (3.1).

Computer animations of the reconstructed dynamics through Equation 5.3 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 cell behind it. 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 Figure 5.9. This type of hopping motion is clearly more noticeable as compared to the small jumps seen in the previous dynamic state of Figure 5.3.

The thickness in the phase-space projections of the POD time coefficients, see Figure 5.8, confirms the presence of stronger temporal modulations as compared to those seen in Figure 5.5. 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 Figure 5.6 are in good agreement with experimental observations of hopping motion [18, 48]. The excursions are governed by modes $\Phi_3$, $\Phi_4$, and $\Phi_5$ of Figure 5.7. Removing these modes (and $\Phi_{10}$ to make the comparison relevant to the states shown in Figure 2.2) we observe a dynamic state with spatio-temporal characteristics as shown in Figure 5.10. The result is strongly similar to those seen in Figure 2.2, especially in column (a).
Figure 5.8: (Top) Phase-space projections produced by the time coefficients of the POD decomposition of the rotating pattern shown in figure 5.6; (bottom) Associated relative phase angles.

Figure 5.9: Reconstruction of the hopping state with $M = 9$ modes.
Figure 5.10: Reconstruction of the hopping state with $M = 9$ modes, excluding modes $\Phi_3, \Phi_4, \text{and } \Phi_5$. 
CHAPTER 6

CONCLUSION AND FURTHER RESEARCH

Understanding the spatio-temporal dynamics of the combustion of premixed gases is an open problem of significant importance to science and industry. Mathematical models have been slow to advance our knowledge of combustion processes due to the interdisciplinary nature of the variables involved and computational complexity. Despite this limitation, laboratory controlled experiments and numerical simulations of certain model equations have been useful in outlining basic features of the dynamics. For instance, these works have shown that premixed gases burn irregularly and form flame patterns through a mechanism that resembles that of reaction-diffusion systems described first by Turing [66].

In order to improve our ability to simulate complex laboratory experiments, it is vital that we make strides to use modern technology to run these simulations. This is especially true in systems that exhibit a sensitive dependence on initial conditions. With these systems, unobservable noise introduced to the experiment could cause the system to cause results to be unrepeatable. Through computer simulation, we are able to control the exact experimental parameters.

In this work, we have numerically discovered a flame pattern that is very common in the laboratory, but has never before been simulated. We have already been able to produce a decomposition to determine the underlying structures that create this state and its unique behavior. This type of flame is common in combustion experiments, and thus in a small way we have enhanced the human ability to simulate these combustion experiments.

In the future we can take advantage of this thesis work to simulate flame patterns a step further, i.e., by introducing an element that is ubiquitous in the real world: noise. By understanding the effect that noise plays on a system that is at a steady state near a bifurcation point we hope to discover other details of flame pattern formation. For instance, we expect to discover more dynamic steady states, common to the laboratory, but less common in numerics. It is also another step closer to better simulate the laboratory environment, and real world results.
BIBLIOGRAPHY


ABSTRACT
ABSTRACT

The motivation for the study of the wide array of complex cellular flame patterns formed on a circular plug burner is to increase the understanding, and be able to suppress, some of these patterns in order to design an efficient burner system. Also, the ability to simulate this very elementary flame type is useful in improving our ability to simulate the real world lab environment. Extended experimental studies in which several complex states have been categorized have been performed [16, 18, 17, 20]. The uniform flame front can be made to undergo symmetry-breaking bifurcations and produce interesting stationary and non-stationary multi-cell patterns. Thus there is a third purpose to our study, to better understand the bifurcation points in the O(2) symmetry group.

We review the basic tools for studying bifurcations using pattern formation. We present an algorithm for the time-integration of nonlinear partial differential equations. The algorithm uses distributed approximating functionals (DAFs), which are based on an analytic approximation method, in order to achieve highly accurate spatial derivatives. The time integration is based on a second order A-stable Crank-Nicolson scheme with a Newton solver.

We present two simulated solutions of the Kuramoto-Sivanshinsky equation on a circular burner. One solution is the first known observation of a numerically generated "hopping" state. The results are decomposed to reveal the details of the bifurcations leading to these states. These results are compared to physical results for verification, and an understanding of the differences.