EFFICIENT COMPUTATIONAL MODELS FOR PATTERN FORMATION IN FIXED AND EVOLVING DOMAINS

by

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ABSTRACT

We efficiently model spatial patterns formed by nonlinear reaction-diffusion equations for benchmark reaction kinetics. Computational methods for modeling reaction-diffusion equations have been presented extensively in literature. Efficiency in these computational methods, either higher convergence or reduced computation time, is desired. We use a moving finite element method presented in literature and adapt it to include a second order convergence discretization and linearization. An algorithm is presented that utilizes these higher convergence methods. Numerical results demonstrate the order of convergence and reduced computational times required to model pattern formation on stationary and time dependent spatial domains. Mode isolation using manipulation of the Turing parameter space is conducted for validation. Pattern evolution on time dependent spatial domains is demonstrated.

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CHAPTER 1

INTRODUCTION

In this thesis we efficiently model spatial patterns that are formed by a system of chemicals that diffuse and react in spatial domains. This spatial pattern formation is studied in the context of biological systems. Spatial pattern formation in biological systems is of interest in the studies of morphogenesis, animal coat markings, predator-prey interactions, and tumor growth to name but a few [3, 4, 5, 7, 16]. In Figures 1.1 and 1.2, we present two examples of spatial patterns in the context of biological systems.

Figure 1.1: Spatial Pattern Expressed as Stripes on a Fish. [1]

Figure 1.2: Spatial Pattern Expressed as Stripes on Zebras. [2]

Systems of reaction-diffusion equations were first used to model spatial pattern formation by Turing in 1953 [16]. Turing's seminal paper used pattern formation in studying morphogenesis, the development of differentiated structure from a homogeneous state [13]. While the reaction kinetics used in Turing's seminal work were linear, which have since been concluded to be too simplistic [11], this work presents diffusion driven spatial pattern formation succinctly. Recent work in modeling biological spatial patterns using reaction-diffusion equations has focused on using nonlinear reaction kinetics and spatial domains that evolve in time [5, 6, 11]. These particular models rely on numerical simulation. Inherent in these numerical schemes is an error in approximate solutions. As current models use nonlinear reaction kinetics, these numerical schemes rely on either nonlinear solvers

or linearization techniques, which can increase either the inherent error or computational time of numeric simulation.

For this thesis our focus is to develop and implement efficient algorithms for the class of nonlinear reaction-diffusion equations that model spatial pattern formation [15, 16]. The algorithms we develop here are more efficient than those presented in the literature [11] due to different discretizations and linearizations. Specifically, we demonstrate that the use of a Crank-Nicolson discretization, in conjunction with a novel linearization, offers order $\mathcal{O}(\triangle t^2)$ convergence and reduced computational time in comparison to a scheme with a low-order nonlinear iterative algebraic system solver at each iterative time step. This higher convergence discretization in conjunction with linearization leads to less computational time to find patterns of a given accuracy or conversly patterns of higher accuracy given similar computational time.

The reaction-diffusion model investigated in this thesis can be written as

$$\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = D\triangle \mathbf{u}(\mathbf{x},t) + \mathbf{f}(\mathbf{u}(\mathbf{x},t)), \qquad (\mathbf{x},t) \in \Omega \times (0,T), \tag{1.1}$$

$$\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial \mathbf{n}(\mathbf{x})} = 0, \qquad \mathbf{x} \in \partial\Omega, \tag{1.2}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{g}(\mathbf{x}), \tag{1.3}$$

where $\mathbf{n}(\mathbf{x})$ is the outward unit normal vector of $\partial\Omega$. We treat $\mathbf{u}(\mathbf{x},t)$ as a vector of two chemical species: $\mathbf{u}(\mathbf{x},t) = [u(\mathbf{x},t), v(\mathbf{x},t)]$. D is a diagonal matrix of diffusion coefficients, $\triangle$ represents the Laplacian, and $\mathbf{f}$ is vector valued function of reaction kinetics. We note that $\Omega \subset \mathbb{R}^n, n = 1,2,3$ is the spatial domain, which can either be fixed or time dependent. We also note that equation (1.2) specifies zero flux boundary conditions on $\partial\Omega$, while equation (1.3) specifies given initial conditions.

This class of nonlinear parabolic partial differential equations (PDE) has been numerically simulated using finite element methods (FEM) in literature [5, 11]. We demonstrate our approach using these examples. Specifically, in modeling pattern formation on a time dependent spatial domain we use a moving FEM described in [5]. This method presents a formulation for temporal derivatives that accommodates a variety of discretizations. More discussion of this method is given in Chapter 4 of this thesis.

The structure of the remainder of this thesis is as follows. Chapter 2 presents the mathematical background of Turing pattern formation as well as the benchmark reaction kinetics. Chapter 3 presents the development of an algorithm to model pattern formation on a fixed spatial domain. Chapter 4 presents the development of an algorithm to model pattern formation on a time dependent spatial domain.

CHAPTER 2

TURING PATTERN FORMATION AND PARAMETER SPACE

Turing pattern formation, also called diffusion driven spatial pattern formation, occurs when a reaction-diffusion system becomes linearly unstable in the presence of diffusion. To define this phenomena, and the range of parameters for which it occurs, we first formulate a generalized reaction-diffusion system. We then present benchmark reaction kinetics for this system. These benchmark kinetics each contain parameters with which we define a space, sometimes called the Turing Space, that facilitates pattern formation. Specifically, we discuss the kinetics and their non-dimensionalization, as the parameters physical meaning and their influence on patterns becomes crucial later in this thesis.

2.1 A General Reaction-Diffusion Model

Here we present motivation for a general reaction-diffusion model for two chemical species following the derivations in literature [5, 11]. To begin, we let $\mathbf{u}(\mathbf{x},t) = [u(\mathbf{x},t), v(\mathbf{x},t)]$ be a vector of two chemical species u, v at a point $\mathbf{x}$ and time t. We treat u, v as concentrations of their respective chemical. We also consider $\mathbf{x} \in \Omega \subset \mathbb{R}^n$ where Ω is the spatial domain and $\partial\Omega$ is the boundary of this spatial domain for $n = 1, 2, 3$. We also let $(0, T) \subset \mathbb{R}$ be the evolutionary time interval, where our intent is to simulate the model for $t \in (0, T)$ given an initial state $\mathbf{u}(\mathbf{x}, 0)$.

Following the literature [11], if we use the law of conservation of mass for $\mathbf{u}(\mathbf{x}, t)$, then we obtain

$$\frac{\partial}{\partial t}\int_V \mathbf{u}\, dV = -\int_{\partial V} (\mathbf{F}\cdot\mathbf{n})\, dS + \int_V \mathbf{f}(\mathbf{u})\, dV\,,$$

where $\mathbf{F}$ is a vector of fluxes for the chemical species, $\mathbf{f}$ is a vector valued function of reaction rates for the chemical species, and $\mathbf{n}$ is the outward unit normal vector to the surface ∂V of an arbitrary volume V. Now, using the divergence theorem yields:

$$\int_V \left(\frac{\partial \mathbf{u}}{\partial t} + \nabla\cdot\mathbf{F} - \mathbf{f}(\mathbf{u})\right) dV = 0\,.$$

Since V was arbitrary, we obtain

$$\frac{\partial \mathbf{u}}{\partial t} = -\nabla\cdot\mathbf{F} + \mathbf{f}(\mathbf{u})\,.$$

Using Fick's law, the flux of a chemical is proportional to the gradient of its concentration, we can further write

$$\frac{\partial \mathbf{u}}{\partial t} = D\nabla^2\mathbf{u} + \mathbf{f}(\mathbf{u})\,, \tag{2.1}$$

which is a standard reaction-diffusion model, with D being a matrix of diffusion coefficients. We note that the diffusion coefficients, entries of D, are assumed to be independent of space and time. Also, typically D is taken as a diagonal matrix, which requires that the chemical species diffuse independently of each other.

Equation (2.1) can be written in matrix form as:

$$\begin{bmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix} \begin{bmatrix} \triangle u \\ \triangle v \end{bmatrix} + \begin{bmatrix} f_1(u,v) \\ f_2(u,v) \end{bmatrix}, \tag{2.2}$$

where $\triangle u = \nabla^2 u$, and d_1, d_2 are parameters.

2.2 Benchmark Reaction Kinetics

In equation (2.1), $\mathbf{f}(\mathbf{u})$ represents a vector valued function of reaction rates for the two chemical species. In [11, 14], several types of reaction kinetics, with various parameters, are used. Two of these kinetics were selected to be benchmark kinetics for our simulations. Below we describe these benchmark kinetic models as well as their non-dimensionalization.

2.2.1 Gierer-Meinhardt Kinetics

The Gierer-Meinhardt reaction kinetics are given by

$$\mathbf{f}(\mathbf{u}) = \begin{bmatrix} f_1(u,v) \\ f_2(u,v) \end{bmatrix},$$
$$f_1(u,v) = k_1 - k_2 u + \frac{k_3 u^2}{v(k_6 + k_7 u^2)}, \quad f_2(u,v) = k_4 u^2 - k_5 v\,,$$

where $k_i, i = 1, \ldots, 7$ are positive real parameters. Substituting these definitions into equation (2.1) allows non-dimensionalization by defining

$$u = U\overline{u}, \quad v = V\overline{v}, \quad t = T\overline{t}, \quad x = L_x\overline{x}\,,$$

where U, V, T are constants, and L_x is a typical length scale for a one dimensional spatial domain.

We notice that the chain rule applied to the partial derivatives yields:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial u}{\partial \overline{t}}\frac{\partial \overline{t}}{\partial t} = \frac{\partial (U\overline{u})}{\partial \overline{t}}\frac{\partial (t/T)}{\partial t} = \left(\frac{U}{T}\right)\frac{\partial \overline{u}}{\partial \overline{t}} = \left(\frac{U}{T}\right)\overline{u}_{\overline{t}}\,, \\ \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial \overline{x}}\frac{\partial \overline{x}}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial (U\overline{u})}{\partial \overline{x}}\frac{\partial (x/L_x)}{\partial x}\right), \\ &= \frac{\partial}{\partial x}\left(\frac{U}{L_x}\frac{\partial \overline{u}}{\partial \overline{x}}\right) = \left(\frac{U}{L_x}\right)\frac{\partial^2 \overline{u}}{\partial \overline{x}^2}\frac{\partial \overline{x}}{\partial x} = \left(\frac{U}{L_x^2}\right)\overline{u}_{\overline{x}\overline{x}}\,. \end{aligned}$$

Thus the Gierer-Meinhardt reaction-diffusion system with these substitutions can be written as

$$\frac{U}{T}\overline{u}_{\overline{t}} = d_1\frac{U}{L_x^2}\triangle\overline{u} + k_1 - k_2U\overline{u} + \frac{k_3U^2\overline{u}^2}{V\overline{v}(k_6 + k_7U^2\overline{u}^2)}\,, \tag{2.3}$$

$$\frac{V}{T}\overline{v}_{\overline{t}} = d_2\frac{V}{L_x^2}\triangle\overline{v} + k_4U^2\overline{u}^2 - k_5V\overline{v}\,. \tag{2.4}$$

Multiplying equation (2.3) by T/U and equation (2.4) by T/V further yields

$$\overline{u}_{\overline{t}} = \frac{Td_1}{L_x^2}\triangle\overline{u} + \frac{Tk_1}{U} - Tk_2\overline{u} + \frac{Tk_3U\overline{u}^2}{k_6V\overline{v}(1+\frac{k_7}{k_6}U^2\overline{u}^2)}\,, \tag{2.5}$$

$$\overline{v}_{\overline{t}} = \frac{Td_2}{L_x^2}\triangle\overline{v} + \frac{Tk_4U^2\overline{u}^2}{V} - Tk_5\overline{v}\,. \tag{2.6}$$

Defining $T = \frac{L_x^2}{d_1}$, and substituting into equations (2.5) and (2.6) leads to

$$\begin{aligned}\overline{u}_{\overline{t}} &= \triangle\overline{u} + \frac{L_x^2k_1}{d_1U} - \frac{L_x^2k_2\overline{u}}{d_1} + \frac{L_x^2k_3U\overline{u}^2}{d_1k_6V\overline{v}(1+\frac{k_7}{k_6}U^2\overline{u}^2)}\,,\\ &= \triangle\overline{u} + \frac{L_x^2}{d_1}\left(\frac{k_1}{U} - k_2\overline{u} + \frac{k_3U\overline{u}^2}{k_6V\overline{v}(1+\frac{k_7}{k_6}U^2\overline{u}^2)}\right)\,,\end{aligned} \tag{2.7}$$

$$\begin{aligned}\overline{v}_{\overline{t}} &= \frac{d_2}{d_1}\triangle\overline{v} + \frac{L_x^2k_4U^2\overline{u}^2}{d_1V} - \frac{L_x^2k_5\overline{v}}{d_1}\,,\\ &= \frac{d_2}{d_1}\triangle\overline{v} + \frac{L_x^2}{d_1}\left(\frac{k_4U^2\overline{u}^2}{V} - k_5\overline{v}\right)\,.\end{aligned} \tag{2.8}$$

Now, we define parameters

$$\begin{aligned}&d = \frac{d_2}{d_1}, \quad \gamma = \frac{L_x^2k_5}{d_1}, \quad U = \frac{k_3}{k_4k_6}, \quad V = \frac{k_3^2}{k_4k_5k_6^2}\,,\\ &a = \frac{k_1k_4k_6}{k_3k_5}, \quad b = \frac{k_2}{k_5}, \quad k = \frac{k_3^2k_7}{k_4^2k_6^3}\,.\end{aligned}$$

Substitution of these parameters into equations (2.7) and (2.8) while dropping the bars for notational simplicity, i.e. $\overline{u} = u$, leads to the non-dimensionalized Gierer-Meinhardt system

$$u_t = \triangle u + \gamma\left(a - bu + \frac{u^2}{v(1+ku^2)}\right)\,, \tag{2.9}$$

$$v_t = d\triangle v + \gamma\left(u^2 - v\right)\,. \tag{2.10}$$

2.2.2 Schnakenberg Reaction Kinetics

The Schnakenberg reaction kinetics are given by

$$\mathbf{f}(\mathbf{u}) = \begin{bmatrix} f_1(u,v) \\ f_2(u,v) \end{bmatrix},$$
$$f_1(u,v) = k_1 a_1 - k_2 u + k_3 u^2 v, \quad f_2(u,v) = k_4 b_1 - k_3 u^2 v\,,$$

where $k_i : i = 1, \ldots, 4$ are positive real parameters, and a_1, b_1 are parameters such that $a_1 \geq 0, b_1 \geq 0$. These equations are non-dimensionalized following the same methodology that we used on the Gierer-Meinhardt kinetics. We define

$$u = U\overline{u}, \quad v = V\overline{v}, \quad t = T\overline{t}, \quad x = L_x\overline{x}\,,$$
$$U = V = \sqrt{\frac{k_2}{k_3}}, \quad T = \frac{L_x^2}{d_1}\,,$$
$$a = \frac{k_1 a_1}{k_2}\sqrt{\frac{k_3}{k_2}}, \quad b = \frac{k_4 b_1}{k_2}\sqrt{\frac{k_3}{k_2}}, \quad \gamma = \frac{k_2 L_x^2}{d_1}, \quad d = \frac{d_2}{d_1}\,.$$

Substitution of these definitions into the reaction-diffusion system (2.1), along with dropping bars for notational simplicity, leads to the non-dimensional system:

$$u_t = \triangle u + \gamma(a - u + u^2 v)\,, \tag{2.11}$$
$$v_t = d\triangle v + \gamma(b - u^2 v)\,. \tag{2.12}$$

2.3 Turing Pattern Formation

In this section we consider the situations in which we observe Turing pattern formation. We consider a generalization of equation (2.2), to represent a non-dimensionalized system for the benchmark reaction kinetics presented earlier:

$$\begin{bmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = \begin{bmatrix} \triangle u \\ d\triangle v \end{bmatrix} + \begin{bmatrix} \gamma f_1(u,v) \\ \gamma f_2(u,v) \end{bmatrix}. \tag{2.13}$$

In the absence of diffusion, consider a homogeneous steady state of equation (2.13), $(u,v) = (u_{hom}, v_{hom})$, such that u_{hom}, and v_{hom} are solutions of $\mathbf{f}(u_{hom}, v_{hom}) = \mathbf{0}$. We also consider a uniform steady state, $(u,v) = (u_s, v_s)$, such that u_s and v_s are constants in both space and time, such that $\mathbf{f}(u_s, v_s) = \mathbf{0}, \triangle u_s = 0, \triangle v_s = 0$. We note that a uniform steady state of equation (2.13) is a homogeneous steady state. More generally, the set of uniform steady states is a subset of the homogeneous steady states.

Turing pattern formation occurs for our reaction-diffusion equation when a homogeneous steady state which is linearly stable in the absence of diffusion, becomes linearly unstable in the presence of diffusion. It is now well documented, [9, 11, 12, 15], that there exist four conditions for the parameters of the reaction kinetics to exhibit Turing pattern formation. Using the notation $f_{nz} = \partial f_n/\partial z$ where these partial derivatives are evaluated at the homogeneous steady state of interest, the four conditions are:

$$\begin{aligned} &f_{1u} + f_{2v} < 0\,, \\ &f_{1u}f_{2v} - f_{1v}f_{2u} > 0\,, \\ &df_{1u} + f_{2v} > 0\,, \\ &(df_{1u} + f_{2v})^2 - 4d\,(f_{1u}f_{2v} - f_{1v}f_{2u}) > 0\,. \end{aligned} \tag{2.14}$$

While we do not present a derivation of these conditions in this thesis, two additional equations of interest surface in their derivation. The first equation of interest determines a critical value for the diffusion coefficient, d_c:

$$d_c^2 f_{1u}^2 + d_c\,(4f_{2u}f_{1v} - 2f_{1u}f_{2v}) + f_{2v}^2 = 0\,, \tag{2.15}$$

and for Turing pattern formation to occur we must have

$$d > d_c\,. \tag{2.16}$$

The second equation of interest allows us to isolate patterns of a specific wavelength using the parameter space. While in practice, in application to biological systems, we would expect many wavelengths to contribute to any pattern, mode isolation serves to verify algorithm development. Here we assume that a spatial pattern modeled by equation (2.13) is composed of modes $\cos(kx)$, $k = n\pi$, $n \in \mathbb{N}$. This assumption is valid for a one dimensional spatial domain of unit length. Given that the four conditions of equation (2.14) hold, and equation (2.16) is also satisfied, we can then predict which modes, which range of wave numbers k, will be excited using

$$(L < k^2 < R),\quad \begin{matrix} L = \frac{\gamma}{2d}\left[(f_{2v} + df_{1u}) - \sqrt{(f_{2v} + df_{1u})^2 - 4d\,|A|}\right] \\ R = \frac{\gamma}{2d}\left[(f_{2v} + df_{1u}) + \sqrt{(f_{2v} + df_{1u})^2 - 4d\,|A|}\right] \end{matrix}\,, \tag{2.17}$$

were

$$|A| = f_{1u}f_{2v} - f_{1v}f_{2u}\,.$$

2.4 Turing Space for Benchmark Kinetics

The four conditions presented in equation (2.14) can be applied to the benchmark reaction kinetics presented earlier in this chapter. Doing so allows us to define the range of parameters, the Turing space, that facilitates pattern formation in spatial domains.

2.4.1 Turing Space: Schnakenberg Kinetics

We recall from equations (2.11) and (2.12) that non-dimensional Schankenberg reaction kinetics are written as

$$\begin{aligned} f_1(u,v) &= a - u + u^2 v\,, \\ f_2(u,v) &= b - u^2 v\,. \end{aligned}$$

Thus, the partial derivatives of these reaction kinetics are given by

$$\begin{aligned} f_{1u} &= -1 + 2uv, \quad f_{1v} = u^2\,, \\ f_{2u} &= -2uv, \quad f_{2v} = -u^2\,. \end{aligned}$$

For equation (2.14) we desire to evaluate these terms at a homogenous steady state. Thus we wish to solve the nonlinear algebraic system $f_1(u_s, v_s) = 0$, $f_2(u_s, v_s) = 0$ for u_s, v_s:

$$\begin{aligned} & a - u_s + u_s^2 v_s = 0, \quad b - u_s^2 v_s = 0\,, \\ \Rightarrow & a - u_s + u_s^2 v_s + b - u_s^2 v_s = a - u_s + b = 0\,, \\ \Rightarrow & u_s = a + b\,, \\ \text{and thus:} \quad & b - (a+b)^2 v_s = 0\,, \\ \Rightarrow & v_s = \frac{b}{(a+b)^2}\,. \end{aligned}$$

Therefore, the four partial derivative terms evaluated at the steady state to use in the conditions are given by:

$$\begin{aligned} f_{1u}|_{(u_s,v_s)} &= -1 + \frac{2b}{a+b}, \quad f_{1v}|_{(u_s,v_s)} = (a+b)^2\,, \\ f_{2u}|_{(u_s,v_s)} &= -\frac{2b}{a+b}, \quad f_{2v}|_{(u_s,v_s)} = -(a+b)^2\,. \end{aligned}$$

With these values substituted into equation (2.14) we obtain the conditions for Turing pattern

formation with Schnakenberg kinetics:

$$\begin{aligned}
&\frac{2b}{a+b} - 1 - (a+b)^2 < 0\,,\\
&\left(-\frac{2b}{a+b} + 1\right)(a+b)^2 + (a+b)^2\left(\frac{2b}{a+b}\right) > 0\,,\\
&d\left(\frac{2b}{a+b} - 1\right) - (a+b)^2 > 0\,,\\
&\left[d\left(\frac{2b}{a+b} - 1\right) - (a+b)^2\right]^2 - 4d\left[\left(-\frac{2b}{a+b} + 1\right)(a+b)^2 + (a+b)^2\left(\frac{2b}{a+b}\right)\right] > 0\,. \qquad (2.18)
\end{aligned}$$

System (2.18) defines the parameter space for (a, b, d) to observe Turing pattern formation. We can algebraically simplify these inequalities, as seen in [15], to yield:

$$\begin{aligned}
&\frac{b-a}{a+b} < (a+b)^2\,,\\
&(a+b)^2 > 0\,,\\
&d\frac{b-a}{a+b} > (a+b)^2\,,\\
&\left[d\left(\frac{b-a}{a+b}\right) - (a+b)^2\right]^2 > 4d(a+b)^2\,. \qquad (2.19)
\end{aligned}$$

Before moving to the other reaction kinetics, if we substitute the parameter values $a = 0.1, b = 0.9$ used in [11], we find the steady state $(u_s, v_s) = (1.0, 0.9)$ and system (2.19) becomes:

$$\begin{aligned}
&0.8 < 1 \quad \Rightarrow True\,,\\
&1 > 0 \quad \Rightarrow True\,,\\
&d(0.8) > 1 \quad \Rightarrow d > 1.25\,,\\
&d^2(0.8^2) - d(5.6) + 1 > 0\,. \qquad (2.20)
\end{aligned}$$

We note that the fourth condition of system (2.20) is identical to equation (2.15) with the relevant derivatives evaluated at the steady state. This fourth condition gives us the critical diffusion coefficient, which can be numerically evaluated as $d > d_c = 8.5676$.

Thus for Schnakenberg kinetics we will have Turing pattern formation with $a = 0.1, b = 0.9, d \geq 8.5677$. Further, we can deduce specific pattern wavelengths by manipulating equation (2.17) .

Fixing $d = 10$, which is consistent with (2.20), we find values of gamma to excite the π mode:

$$
\begin{aligned}
&L = \gamma\frac{4}{20} = \frac{\gamma}{5}\,,\\
&R = \gamma\frac{10}{20} = \frac{\gamma}{2}\,,\\
&L < (1^2)\pi^2 < R \;\rightarrow\; \frac{\gamma}{5} < \pi^2 < \frac{\gamma}{2}\,,\\
&\rightarrow \gamma < 5\pi^2 \approx 49.348,\; \gamma > 2\pi^2 \approx 19.739\,.
\end{aligned}
$$

For other pattern wavelengths, we similarly manipulate equation (2.17). We summarize the findings in Table 2.1 .

Table 2.1: Values of γ for Pattern Wavelengths: Schnakenberg Kinetics

k^2	γ_{min}	γ_{max}
$(\pi)^2$	19.739	49.348
$(2\pi)^2$	78.957	179.392
$(3\pi)^2$	177.652	444.132
$(4\pi)^2$	315.827	789.568

We note that the values from Table 2.1 match well with those given in [11, Page 37]. Also as an aside, equation (2.19) presents the parameter space explicitly in terms of parameters a, b from the Schnakenberg kinetics. This is due to finding the uniform steady state analytically in this case. It is however noted in the literature [12], that "Except for simple mechanisms these cannot be found analytically with ease...". Thus the Turing space is presented in numeric rather then analytic inequalities for Gierer-Meinhardt kinetics.

2.4.2 Turing Space: Gierer-Meinhardt Kinetics

In this section we numerically verify the Turing space for parameter choices given in literature [11, 15]. We recall from equations (2.9) and (2.10) that Gierer-Meinhardt reaction kinetics are written non-dimensionally as

$$
\begin{aligned}
f_1(u,v) &= a - bu + \frac{u^2}{v(1+ku^2)}\,,\\
f_2(u,v) &= u^2 - v\,.
\end{aligned}
$$

We find the partial derivatives of these reaction kinetics as

$$\begin{aligned} f_{1u} &= -b + \frac{2u}{v(1+ku^2)^2}, \quad f_{1v} = \frac{-u^2}{v^2(1+ku^2)}\,, \\ f_{2u} &= 2u, \quad f_{2v} = -1\,. \end{aligned} \tag{2.21}$$

Using parameter values of $a = 0.1, b = 1, k = 0.5$, as seen in [11, 15], we obtain

$$\begin{aligned} f_1(u,v) &= 0.1 - u + \frac{u^2}{v(1+0.5u^2)}\,, \\ f_2(u,v) &= u^2 - v\,. \end{aligned}$$

Thus the steady state (u_s, v_s) satisfying $f_1(u_s, v_s) = 0 = f_2(u_s, v_s)$ is given by.

$$\begin{aligned} v_s =& u_s^2\,, \\ 0 =& 0.1 - u_s + \frac{u_s^2}{u_s^2(1+0.5u_s^2)}\,. \end{aligned} \tag{2.22}$$

Numerically solving system (2.22) yields:

$$u_s \approx 0.8394569, \quad v_s \approx 0.7046878\,.$$

With these numeric solutions plugged into the partials derivatives, equation (2.21), we obtain

$$\begin{aligned} f_{1u}|_{(u_s,v_s)} &= 0.3027387\,, \\ f_{1v}|_{(u_s,v_s)} &= -1.0493396\,, \\ f_{2u}|_{(u_s,v_s)} &= 1.6789137\,, \\ f_{2v}|_{(u_s,v_s)} &= -1\,. \end{aligned} \tag{2.23}$$

We verify that these parameter choices facilitate Turing pattern formation using the conditions of system (2.14):

$$\begin{aligned} &-0.6972613 < 0 \Rightarrow True\,, \\ &1.4590120 > 0 \Rightarrow True\,, \\ &d(0.3027387) - 1 > 0 \Rightarrow d > 3.3031790\,, \\ &(d(0.3027387) - 1)^2 - 4d(1.4590120) > 0\,. \end{aligned} \tag{2.24}$$

The last line of system (2.24) is equivalent to finding the d_c value, in equation (2.15), for these parameter choices. We obtain $d > d_c \approx 70.1278$. As with Schnakenberg kinetics, we can use

equation (2.17) to predict gamma values for specific wavelength excitation. Fixing $d = 72$ which is consistent with system (2.24), we find values of gamma to excite specific pattern wavelengths:

$$
\begin{aligned}
L &= \frac{\gamma}{144}\,(17.2861) = \gamma(0.1200)\,, \\
R &= \frac{\gamma}{144}(24.3082) = \gamma(0.1688)\,, \\
L &< (1^2)\pi^2 < R \;\rightarrow\; \gamma(0.1200) < \pi^2 < \gamma(0.1688)\,, \\
&\Rightarrow \gamma < \frac{\pi^2}{0.1200} \approx 82.217,\; \gamma > \frac{\pi^2}{0.1688} \approx 58.467\,.
\end{aligned}
$$

For other wavelengths, we similarly manipulate equation (2.17). We summarize the findings in Table 2.2 .

Table 2.2: Values of γ for Pattern Wavelengths: Gierer-Meinhardt Kinetics

k^2	γ_{min}	γ_{max}
$(\pi)^2$	58.467	82.217
$(2\pi)^2$	233.867	328.870
$(3\pi)^2$	526.201	739.960
$(4\pi)^2$	935.468	1315.479

We note that the values presented in Table 2.2 match well with those presented in [11]. With the parameter spaces for Turing pattern formation enumerated for our benchmark kinetics, we next discuss the development of the algorithm to model this pattern formation on a fixed spatial domain.

CHAPTER 3

PATTERN FORMATION ON A FIXED DOMAIN

In this chapter we develop an algorithm to model pattern development on fixed spatial domains. Our algorithm uses a finite element method and includes two choices of discretization and linearization. For the discretization we use the Backward Euler and the Crank-Nicolson methods. Both discretizations are used in conjunction with efficient linearizations.

For this chapter, we use as the core mathematical model a dimensionless reaction-diffusion equation in two chemical species, u, v, with zero flux boundary conditions and given initial conditions:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \gamma f_1(u,v), \qquad (x,t) \in (\alpha,\beta) \times (0,T)\,, \tag{3.1}$$

$$\frac{\partial v}{\partial t} = d\frac{\partial^2 v}{\partial x^2} + \gamma f_2(u,v), \qquad (x,t) \in (\alpha,\beta) \times (0,T)\,, \tag{3.2}$$

$$\frac{\partial u(\alpha,t)}{\partial x} = \frac{\partial u(\beta,t)}{\partial x} = \frac{\partial v(\alpha,t)}{\partial x} = \frac{\partial v(\beta,t)}{\partial x} = 0, \qquad t \in (0,T)\,, \tag{3.3}$$

$$u(x,0) = g_1(x),\ v(x,0) = g_2(x), \qquad x \in (\alpha,\beta)\,, \tag{3.4}$$

where $f_1(u,v)$, $f_2(u,v)$ are reaction kinetics given in Chapter 2. In order to establish a finite element method for this model we first describe the variational formulation.

3.1 Variational Formulation

A finite element method to numerically simulate equations (3.1) and (3.2) begins with a variational formulation. For our continuous model, we seek each component solution in the standard Sobolev space $\mathcal{V} = H^1(\alpha,\beta)$, comprising all weakly differentiable functions on (α,β). Then, to find the variational formulation of equations (3.1) and (3.2) we multiply each by a test function $w \in \mathcal{V}$ and integrate over the spatial domain $x \in (\alpha,\beta)$:

$$\int_\alpha^\beta \frac{\partial u}{\partial t} w - \int_\alpha^\beta \frac{\partial^2 u}{\partial x^2} w - \int_\alpha^\beta \gamma f_1(u,v) w = 0\,,\ \forall w \in \mathcal{V}\,, \tag{3.5}$$

$$\int_\alpha^\beta \frac{\partial v}{\partial t} w - \int_\alpha^\beta d\frac{\partial^2 v}{\partial x^2} w - \int_\alpha^\beta \gamma f_2(u,v) w = 0\,,\ \forall w \in \mathcal{V}\,. \tag{3.6}$$

We now consider the boundary conditions, equation (3.3). Using equation (3.3) and integration

by parts for equations (3.5) and (3.6) yields,

$$\begin{aligned}
\int_\alpha^\beta \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) w &= \frac{\partial u}{\partial x} w\Big|_\alpha^\beta - \int_\alpha^\beta \frac{\partial u}{\partial x}\frac{\partial w}{\partial x}\,, \\
&= \frac{\partial u(\beta,t)}{\partial x} w(\beta) - \frac{\partial u(\alpha,t)}{\partial x} w(\alpha) - \int_\alpha^\beta \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = -\int_\alpha^\beta \frac{\partial u}{\partial x}\frac{\partial w}{\partial x}\,, \\
\int_\alpha^\beta d\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x}\right) w &= d\,\frac{\partial v}{\partial x} w\Big|_\alpha^\beta - d\int_\alpha^\beta \frac{\partial v}{\partial x}\frac{\partial w}{\partial x}\,, \\
&= d\frac{\partial v(\beta,t)}{\partial x} w(\beta) - d\frac{\partial v(\alpha,t)}{\partial x} w(\alpha) - d\int_\alpha^\beta \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = -d\int_\alpha^\beta \frac{\partial v}{\partial x}\frac{\partial w}{\partial x}\,.
\end{aligned}$$

With these simplifications applied to equations (3.5) and (3.6) we obtain the weak-form system

$$\int_\alpha^\beta \frac{\partial u}{\partial t} w + \int_\alpha^\beta \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = \int_\alpha^\beta \gamma f_1(u,v) w, \quad \forall w \in \mathcal{V}\,, \tag{3.7}$$

$$\int_\alpha^\beta \frac{\partial v}{\partial t} w + d\int_\alpha^\beta \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = \int_\alpha^\beta \gamma f_2(u,v) w, \quad \forall w \in \mathcal{V}\,. \tag{3.8}$$

The system (3.7)-(3.8) is the variational formulation for equations (3.1)-(3.3).

3.2 Finite Element Method: Schnakenberg Kinetics

In this section we describe the discretizations, both Backward Euler and Crank-Nicolson, and linearizations that enable us to write the variational formulation in a finite dimensional space $\mathcal{V}_h$, as a linear system at each discrete time step. Specifically, we address with the variational formulation with Schnakenberg kinetics in this section. The variational formulation of interest is thus:

$$\int_\alpha^\beta \frac{\partial u}{\partial t} w + \int_\alpha^\beta \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = \int_\alpha^\beta \gamma(a - u + u^2 v) w, \quad \forall w \in \mathcal{V}\,, \tag{3.9}$$

$$\int_\alpha^\beta \frac{\partial v}{\partial t} w + d\int_\alpha^\beta \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = \int_\alpha^\beta \gamma(b - u^2 v) w, \quad \forall w \in \mathcal{V}\,. \tag{3.10}$$

In order to apply discretizations we establish meshes of the spatial domain and temporal interval. We define,

$$\begin{aligned}
&h = \frac{\beta - \alpha}{N},\ N \in \mathbb{N}\,, \\
&x_1 = \alpha, \quad x_{N+1} = \beta, \quad x_i = x_{i-1} + h,\ i \in \{2, 3, \ldots, N+1\}\,, \\
&\triangle t = \frac{T}{M},\ M \in \mathbb{N}\,, \\
&t_1 = 0, \quad t_{M+1} = T, \quad t_m = (m-1)\triangle t,\ m \in \{2, 3, \ldots, M+1\}\,,
\end{aligned}$$

where $(N+1)$, $(M+1)$ are the number of nodes of the spatial and temporal meshes respectively. We note that a uniform mesh of the spatial domain is used for simplicity in derivation, but non-uniform meshes can be used as well in our algorithm. Using the spatial mesh, we define a $N+1$ dimensional subspace $\mathcal{V}_h \subset \mathcal{V}$:

$$\mathcal{V}_h = \text{Span}\{\phi_i : i = 1, 2, 3, \ldots, N+1\}\,,$$

where ϕ_i is the i^{th} basis function of $\mathcal{V}_h$. These basis functions are defined with support only on subsets of the spatial domain. The subintervals of the spatial domain are denoted as

$$I_i = [x_i, x_{i+1}], \quad i \in \{1, 2, \ldots, N\}\,.$$

We define the basis functions of $\mathcal{V}_h$:

$$\phi_1(x) = \begin{cases} \frac{x_2 - x}{h} & , \quad x \in I_1 \\ 0 & , \quad \text{otherwise} \end{cases},$$

$$\phi_i(x) = \begin{cases} \frac{x - x_{i-1}}{h} & , \quad x \in I_{i-1} \\ \frac{x_{i+1} - x}{h} & , \quad x \in I_i \\ 0 & , \quad \text{otherwise} \end{cases} , \quad i = 2, 3, \ldots, N\,,$$

$$\phi_{N+1}(x) = \begin{cases} \frac{x - x_N}{h} & , \quad x \in I_N \\ 0 & , \quad \text{otherwise} \end{cases}.$$

The FEM approximations u_h, v_h to u, v are sought in $\mathcal{V}_h$. We also define

$$U^m(x) = u_h(x, t_m), \quad V^m(x) = v_h(x, t_m),\ m = 1, 2, \ldots, M+1\,,$$
$$< f, g >= \int_\alpha^\beta f(x) g(x)\, dx, \quad \mathcal{A}(f, g) = \int_\alpha^\beta \frac{\partial f(x)}{\partial x} \frac{\partial g(x)}{\partial x}\, dx\,.$$

3.2.1 Backward Euler Finite Element Method

The Backward Euler FEM for the system (3.9)-(3.10) is given by

$$\left\langle \frac{U^m - U^{m-1}}{\triangle t}, w \right\rangle + \mathcal{A}(U^m, w) = \left\langle \gamma(a - U^m + (U^m)^2 V^m), w \right\rangle\,, \tag{3.11}$$

$$\left\langle \frac{V^m - V^{m-1}}{\triangle t}, w \right\rangle + d\mathcal{A}(V^m, w) = \left\langle \gamma(b - (U^m)^2 V^m), w \right\rangle\,, \tag{3.12}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for}\, m = 2, 3, \ldots, M+1\,.$$

We also approximate the given initial value data g_1, g_2 respectively by U^1, $V^1 \in \mathcal{V}_h$. The bilinear forms $< \cdot, \cdot >$ and $\mathcal{A}$ allow simplification of equations (3.11) and (3.12):

$$(1+\gamma\triangle t)\left\langle U^m, w\right\rangle + \triangle t\mathcal{A}(U^m, w) - \gamma\triangle t\left\langle (U^m)^2 V^m, w\right\rangle = \gamma\triangle t\left\langle a, w\right\rangle + \left\langle U^{m-1}, w\right\rangle , \tag{3.13}$$

$$\left\langle V^m, w\right\rangle + d\triangle t\mathcal{A}(V^m, w) + \gamma\triangle t\left\langle (U^m)^2 V^m, w\right\rangle = \gamma\triangle t\left\langle b, w\right\rangle + \left\langle V^{m-1}, w\right\rangle , \tag{3.14}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for } m = 2, 3, \ldots, M+1 .$$

As opposed to using nonlinear solution techniques, Newton's method for example, we linearize the $(U^m)^2$ terms of equations (3.13) and (3.14) using the approximation $(U^m)^2 \approx \left(U^{m-1}\right)^2$. This approximation can be shown, using the Taylor expansion, to be $\mathcal{O}(\triangle t)$ accurate:

$$u(x, t_{m-1}) = u(x, t_m) - \frac{\partial u(x, t_m)}{\partial t}\triangle t + \left(\frac{1}{2}\right)\frac{\partial^2 u(x, t_m)}{\partial t^2}(\triangle t)^2 + \mathcal{O}(\triangle t^3) = u(x, t_m) + \mathcal{O}(\triangle t) .$$

Equations (3.13) and (3.14) with this linearization can be written as

$$(1+\gamma\triangle t)\left\langle U^m, w\right\rangle + \triangle t\mathcal{A}(U^m, w) = \gamma\triangle t\left\langle (U^{m-1})^2 V^m, w\right\rangle + \gamma\triangle t\left\langle a, w\right\rangle + \left\langle U^{m-1}, w\right\rangle , \tag{3.15}$$

$$\left\langle V^m, w\right\rangle + d\triangle t\mathcal{A}(V^m, w) + \gamma\triangle t\left\langle (U^{m-1})^2 V^m, w\right\rangle = \gamma\triangle t\left\langle b, w\right\rangle + \left\langle V^{m-1}, w\right\rangle , \tag{3.16}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for } m = 2, 3, \ldots, M+1 .$$

Next, the hat basis functions of $\mathcal{V}_h$ allow us to use the representations

$$U^m(x) = \sum_{i=1}^{N+1} k_i^m \phi_i(x), \quad k_i^m \in \mathbb{R} ,$$

$$V^m(x) = \sum_{i=1}^{N+1} l_i^m \phi_i(x), \quad l_i^m \in \mathbb{R} ,$$

where the constants k_i, l_i are unknowns that we wish to solve for. We now substitute the linear combinations of basis functions into equations (3.15) and (3.16). We also notice that equations (3.15) and (3.16) hold for all $w \in \mathcal{V}_h = \text{Span}\{\phi_i : i = 1, 2, \ldots, N+1\}$. Therefore it is sufficient for us replace w in equations (3.15) and (3.16) with ϕ_j, $j = 1, \cdots, N+1$. Thus we obtain:

$$(1+\gamma\triangle t)\sum_{i=1}^{N+1} k_i^m \langle \phi_i, \phi_j\rangle + \triangle t \sum_{i=1}^{N+1} k_i^m \mathcal{A}(\phi_i,\phi_j)$$

$$= \gamma\triangle t \langle a, \phi_j\rangle + \gamma\triangle t \left\langle \left(\sum_{i=1}^{N+1} k_i^{m-1}\phi_i\right)^2 \sum_{i=1}^{N+1} l_i^m \phi_i, \phi_j \right\rangle + \sum_{i=1}^{N+1} k_i^{m-1}\langle \phi_i,\phi_j\rangle \ , \tag{3.17}$$

$$\sum_{i=1}^{N+1} l_i^m \langle \phi_i,\phi_j\rangle + d\triangle t \sum_{i=1}^{N+1} l_i^m \mathcal{A}(\phi_i,\phi_j) + \gamma\triangle t \left\langle \left(\sum_{i=1}^{N+1} k_i^{m-1}\phi_i\right)^2 \sum_{i=1}^{N+1} l_i^m \phi_i, \phi_j \right\rangle$$

$$= \gamma\triangle t \langle b, \phi_j\rangle + \sum_{i=1}^{N+1} l_i^{m-1}\langle \phi_i,\phi_j\rangle \ , \tag{3.18}$$

for $j = 1, 2, \ldots, N+1$, $m = 2, 3, \ldots, M+1$.

We next define the following matrices and vectors

$$[A]_{i,j} = \mathcal{A}(\phi_i,\phi_j), \quad [M]_{i,j} = \langle \phi_i,\phi_j\rangle, \quad [Q^m]_{i,j} = \left\langle \phi_i(\sum_{r=1}^{N+1} k_r^{m-1}\phi_r \sum_{s=1}^{N+1} k_s^{m-1}\phi_s), \phi_j \right\rangle ,$$

$$\mathbf{k^m} = [k_1^m \quad k_2^m \quad \ldots \quad k_{N+1}^m]^T, \quad \mathbf{l^m} = [l_1^m \quad l_2^m \quad \ldots \quad l_{N+1}^m]^T ,$$

$$\mathbf{z_1} = [\langle a,\phi_1\rangle \quad \langle a,\phi_2\rangle \quad \ldots \langle a,\phi_{N+1}\rangle]^T, \quad \mathbf{z_2} = [\langle b,\phi_1\rangle \quad \langle b,\phi_2\rangle \quad \ldots \langle b,\phi_{N+1}\rangle]^T .$$

Using these matrix and vector definitions we represent equations (3.17)-(3.18) as

$$[(1+\gamma\triangle t)\, M + \triangle t A]\, \mathbf{k^m} = (\gamma\triangle t)\mathbf{z_1} + (\gamma\triangle t) Q^m \mathbf{l^m} + M\mathbf{k^{m-1}} , \tag{3.19}$$

$$[M + d\triangle t A + (\gamma\triangle t) Q^m]\, \mathbf{l^m} = (\gamma\triangle t)\mathbf{z_2} + M\mathbf{l^{m-1}}, \quad m = 2, 3, \ldots, M+1 . \tag{3.20}$$

Equations (3.19) and (3.20) constitute a linear system for the unknowns k_i^m, l_i^m, $i = 1, 2, \ldots, N+1$. When these coefficients are solved for, we have the FEM approximation to u, v at a given time t_m, $m = 2, 3, \ldots, M+1$. To implement this system we enumerate matrix entries. Matrices A and M are typical for a FEM, and consequently entries are easily found, [10] :

$$A = \begin{bmatrix} \frac{1}{h_1} & \frac{-1}{h_1} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \frac{-1}{h_{i-1}} & \frac{1}{h_{i-1}} + \frac{1}{h_i} & \frac{-1}{h_i} & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & \frac{-1}{h_N} & \frac{1}{h_N} \end{bmatrix} ,$$

$$M = \begin{bmatrix} \frac{h_1}{3} & \frac{h_1}{6} & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \frac{h_{i-1}}{6} & \frac{h_{i-1}}{3} + \frac{h_i}{3} & \frac{h_i}{6} & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & \frac{h_N}{6} & \frac{h_N}{6} \end{bmatrix}.$$

Elements of the Q^m matrix are not standard for most FEM. We derive the entries as

$$\begin{aligned}
[Q^m]_{i,i} &= \int_{x_{i-1}}^{x_i} (\phi_i)^2 (k_{i-1}^{m-1}\phi_{i-1} + k_i^{m-1}\phi_i)^2 \\
&+ \int_{x_i}^{x_{i+1}} (\phi_i)^2 (k_i^{m-1}\phi_i + k_{i+1}^{m-1}\phi_{i+1})^2,\ i = 2, 3, \ldots, N\,, \\
[Q^m]_{i,i-1} &= \int_{x_{i-1}}^{x_i} (\phi_i)(\phi_{i-1})(k_{i-1}^{m-1}\phi_{i-1} + k_i^{m-1}\phi_i)^2,\ i = 2, 3, \ldots, N\,, \\
[Q^m]_{i,i+1} &= \int_{x_i}^{x_{i+1}} (\phi_i)(\phi_{i+1})(k_i^{m-1}\phi_i + k_{i+1}^{m-1}\phi_{i+1})^2,\ i = 2, 3, \ldots, N\,, \\
[Q^m]_{1,1} &= \int_{x_1}^{x_2} (\phi_1)^2 (k_1^{m-1}\phi_1 + k_2^{m-1}\phi_2)^2\,, \\
[Q^m]_{1,2} &= \int_{x_1}^{x_2} (\phi_1)(\phi_2)(k_1^{m-1}\phi_1 + k_2^{m-1}\phi_2)^2\,, \\
[Q^m]_{N+1,N} &= \int_{x_N}^{x_{N+1}} (\phi_N)(\phi_{N+1})(k_N^{m-1}\phi_N + k_{N+1}^{m-1}\phi_{N+1})^2\,, \\
[Q^m]_{N+1,N+1} &= \int_{x_N}^{x_{N+1}} (\phi_{N+1})^2 (k_N^{m-1}\phi_N + k_{N+1}^{m-1}\phi_{N+1})^2\,.
\end{aligned}$$

These integrals when computed in Mathematica yield:

$$\begin{aligned}
[Q^m]_{1,1} &= \frac{h_1}{30}(6(k_1^{m-1})^2 + 3k_1^{m-1}k_2^{m-1} + (k_2^{m-1})^2))\,, \\
[Q^m]_{1,2} &= \frac{h_1}{60}(3(k_1^{m-1})^2 + 4k_1^{m-1}k_2^{m-1} + 3(k_2^{m-1})^2))\,, \\
[Q^m]_{i,i-1} &= \frac{h_{i-1}}{60}(3(k_{i-1}^{m-1})^2 + 4k_{i-1}^{m-1}k_i^{m-1} + 3(k_i^{m-1})^2)\,, \\
[Q^m]_{i,i} &= \frac{h_{i-1}}{30}((k_{i-1}^{m-1})^2 + 3k_{i-1}^{m-1}k_i^{m-1}) + \frac{h_i}{30}((k_{i+1}^{m-1})^2 + 3k_i^{m-1}k_{i+1}^{m-1})) \\
&+ \frac{(h_{i-1} + h_i)}{30} 6(k_i^{m-1})^2\,, \\
[Q^m]_{i,i+1} &= \frac{h_i}{60}(3(k_i^{m-1})^2 + 4k_i^{m-1}k_{i+1}^{m-1} + 3(k_{i+1}^{m-1})^2)\,, \\
[Q^m]_{N+1,N} &= \frac{h_N}{60}(3(k_N^{m-1})^2 + 4k_N^{m-1}k_{N+1}^{m-1} + 3(k_{N+1}^{m-1})^2)\,, \\
[Q^m]_{N+1,N+1} &= \frac{h_N}{30}((k_N^{m-1})^2 + 3k_N^{m-1}k_{N+1}^{m-1} + 6(k_{N+1}^{m-1})^2)\,.
\end{aligned}$$

An $\mathcal{O}(\triangle t + h^2)$ algorithm that uses equations (3.19) and (3.20) to simulate pattern formation

on a fixed domain has been implemented. Examples of this algorithm's results are presented later in this chapter.

3.2.2 Crank-Nicolson Finite Element Method

A Crank-Nicolson FEM for equations (3.9) and (3.10) is given by

$$\left\langle \frac{U^m - U^{m-1}}{\triangle t}, w \right\rangle + \mathcal{A}(U^{m-1/2}, w) = \left\langle \gamma(a - U^{m-1/2} + (U^{m-1/2})^2 V^{m-1/2}), w \right\rangle , \tag{3.21}$$

$$\left\langle \frac{V^m - V^{m-1}}{\triangle t}, w \right\rangle + d\mathcal{A}(V^{m-1/2}, w) = \left\langle \gamma(b - (U^{m-1/2})^2 V^{m-1/2}), w \right\rangle , \tag{3.22}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for } m = 2, 3, \ldots, M+1 ,$$

where we use the notations

$$U^{m-1/2} = \frac{U^m + U^{m-1}}{2}, \quad V^{m-1/2} = \frac{V^m + V^{m-1}}{2} .$$

We again note that the initial conditions, equation (3.4), determine the approximations $U^1, V^1 \in \mathcal{V}_h$. To simplify equations (3.21) and (3.22) we note the bilinearity of $< \cdot, \cdot >$ and $\mathcal{A}$. After grouping we obtain

$$\begin{aligned} &(1 + \frac{\gamma\triangle t}{2}) \langle U^m, w \rangle + \frac{\triangle t}{2}\mathcal{A}(U^m, w) = (1 - \frac{\gamma\triangle t}{2}) \langle U^{m-1}, w \rangle \\ &- \frac{\triangle t}{2}\mathcal{A}(U^{m-1}, w) + (\gamma\triangle t) \langle a, w \rangle + (\gamma\triangle t) \left\langle (U^{m-1/2})^2 \frac{V^m + V^{m-1}}{2}, w \right\rangle , \end{aligned} \tag{3.23}$$

$$\begin{aligned} &\langle V^m, w \rangle + \frac{d\triangle t}{2}\mathcal{A}(V^m, w) = \langle V^{m-1}, w \rangle - \frac{d\triangle t}{2}\mathcal{A}(V^{m-1}, w) \\ &+ (\gamma\triangle t) \langle b, w \rangle - (\gamma\triangle t) \left\langle (U^{m-1/2})^2 \frac{V^m + V^{m-1}}{2}, w \right\rangle , \end{aligned} \tag{3.24}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for } m = 2, 3, \ldots, M+1 .$$

As opposed to using nonlinear solution techniques for these equations, we use the following linearization for the $(U^{m-1/2})^2$ terms:

$$(U^{m-1/2})^2 \approx \left(\frac{3U^{m-1} - U^{m-2}}{2} \right)^2 .$$

This linearization can be shown, using the Taylor expansion, to be $\mathcal{O}(\triangle t^2)$ accurate:

$$\frac{3u(x,t_{m-1})-u(x,t_{m-2})}{2}=\left(\frac{3}{2}-\frac{1}{2}\right)u(x,t_{m-1/2})+\left(\frac{-3}{4}+\frac{3}{4}\right)\frac{\partial u(x,t_{m-1/2})}{\partial t}\triangle t$$
$$+\left(\frac{3}{16}-\frac{9}{16}\right)\frac{\partial^2 u(x,t_{m-1/2})}{\partial t^2}(\triangle t)^2+\mathcal{O}(\triangle t^3)=u(x,t_{m-1/2})+\mathcal{O}(\triangle t^2)\,.$$

With this linearization applied to equations (3.23) and (3.24), we obtain

$$(1+\frac{\gamma\triangle t}{2})\langle U^m,w\rangle+\frac{\triangle t}{2}\mathcal{A}(U^m,w)=(1-\frac{\gamma\triangle t}{2})\left\langle U^{m-1},w\right\rangle-\frac{\triangle t}{2}\mathcal{A}(U^{m-1},w)$$
$$+(\gamma\triangle t)\langle a,w\rangle+\frac{\gamma\triangle t}{8}\left\langle(9(U^{m-1})^2-6U^{m-1}U^{m-2}+(U^{m-2})^2)(V^m+V^{m-1}),w\right\rangle\,, \tag{3.25}$$
$$\langle V^m,w\rangle+\frac{d\triangle t}{2}\mathcal{A}(V^m,w)=\left\langle V^{m-1},w\right\rangle-\frac{d\triangle t}{2}\mathcal{A}(V^{m-1},w)$$
$$+(\gamma\triangle t)\langle b,w\rangle-\frac{\gamma\triangle t}{8}\left\langle(9(U^{m-1})^2-6U^{m-1}U^{m-2}+(U^{m-2})^2)(V^m+V^{m-1}),w\right\rangle\,, \tag{3.26}$$
$$\forall w\in\mathcal{V}_h,\quad \text{for}\, m=3,4,\ldots,M+1\,.$$

We note that the linearization restricts equations (3.25) and (3.26) to $m\in\{3,4,\ldots,M+1\}$. To solve for the $m=2$ time step we use the following predictor-corrector scheme. Let $X^1=U^1, Y^1=V^1$, then:

$$\left\langle\frac{X^2-X^1}{\triangle t},w\right\rangle+\mathcal{A}\left(\frac{X^2+X^1}{2},w\right)=\left\langle\gamma(a-X^1+(X^1)^2Y^1),w\right\rangle\,,$$
$$\left\langle\frac{Y^2-Y^1}{\triangle t},w\right\rangle+\mathcal{A}\left(d\frac{Y^2+Y^1}{2},w\right)=\left\langle\gamma(b-(X^1)^2Y^1),w\right\rangle\,, \tag{3.27}$$
$$\left\langle\frac{U^2-U^1}{\triangle t},w\right\rangle+\mathcal{A}\left(\frac{U^2+U^1}{2},w\right)=\left\langle\gamma(a-X^{3/2}+(X^{3/2})^2Y^{3/2})),w\right\rangle\,,$$
$$\left\langle\frac{V^2-V^1}{\triangle t},w\right\rangle+\mathcal{A}\left(d\frac{V^2+V^1}{2},w\right)=\left\langle\gamma(b-(X^{3/2})^2Y^{3/2}),w\right\rangle\,, \tag{3.28}$$

where $X^{3/2}=(X^2+X^1)/2$, $Y^{3/2}=(Y^2+Y^1)/2$.

We return to equations (3.25) and (3.26) currently, as the predictor-corrector systems are addressed later in this section. Using the basis functions of $\mathcal{V}_h$, we can write

$$U^m=\sum_{i=1}^{N+1}k_i^m\phi_i,\quad k_i^m\in\mathbb{R}\,,$$
$$V^m=\sum_{i=1}^{N+1}l_i^m\phi_i,\quad l_i^m\in\mathbb{R}\,.$$

We next substitute these linear combinations of basis functions into equations (3.25) and (3.26). We also notice these equations hold for all $w\in\mathcal{V}_h=\text{Span}\{\phi_i:i=1,2,\ldots,N+1\}$. Therefore, it

is sufficient that we replace w in equations (3.25) and (3.26) with ϕ_j, $j = 1, \cdots, N+1$. Thus we obtain:

$$
\begin{aligned}
&(1+\frac{\gamma\triangle t}{2})\sum_{i=1}^{N+1} k_i^m \langle \phi_i, \phi_j\rangle + \frac{\triangle t}{2}\sum_{i=1}^{N+1} k_i^m \mathcal{A}(\phi_i,\phi_j) = (1-\frac{\gamma\triangle t}{2})\sum_{i=1}^{N+1} k_i^{m-1}\langle \phi_i,\phi_j\rangle \\
&-\frac{\triangle t}{2}\sum_{i=1}^{N+1} k_i^{m-1}\mathcal{A}(\phi_i,\phi_j) + \gamma\triangle t\langle a,\phi_j\rangle \\
&+\frac{\gamma\triangle t}{8}\left(\left\langle 9(\sum_{i=1}^{N+1} k_i^{m-1}\phi_i)^2 \sum_{i=1}^{N+1} l_i^m\phi_i,\phi_j\right\rangle - \left\langle 6\sum_{i=1}^{N+1} k_i^{m-1}\phi_i \sum_{i=1}^{N+1} k_i^{m-2}\phi_i \sum_{i=1}^{N+1} l_i^m\phi_i,\phi_j\right\rangle\right. \\
&+\left\langle (\sum_{i=1}^{N+1} k_i^{m-2}\phi_i)^2 \sum_{i=1}^{N+1} l_i^m\phi_i,\phi_j\right\rangle + \left\langle 9(\sum_{i=1}^{N+1} k_i^{m-1}\phi_i)^2 \sum_{i=1}^{N+1} l_i^{m-1}\phi_i,\phi_j\right\rangle \\
&\left.-\left\langle 6\sum_{i=1}^{N+1} k_i^{m-1}\phi_i \sum_{i=1}^{N+1} k_i^{m-2}\phi_i \sum_{i=1}^{N+1} l_i^{m-1}\phi_i,\phi_j\right\rangle + \left\langle (\sum_{i=1}^{N+1} k_i^{m-2}\phi_i)^2 \sum_{i=1}^{N+1} l_i^{m-1}\phi_i,\phi_j\right\rangle\right), \qquad (3.29)\\
&\sum_{i=1}^{N+1} l_i^m\langle \phi_i,\phi_j\rangle + \frac{d\triangle t}{2}\sum_{i=1}^{N+1} l_i^m\mathcal{A}(\phi_i,\phi_j) = \sum_{i=1}^{N+1} l_i^{m-1}\langle \phi_i,\phi_j\rangle - \frac{d\triangle t}{2}\sum_{i=1}^{N+1} l_i^{m-1}\mathcal{A}(\phi_i,\phi_j) \\
&+\gamma\triangle t\langle b,\phi_j\rangle \\
&-\frac{\gamma\triangle t}{8}\left(\left\langle 9(\sum_{i=1}^{N+1} k_i^{m-1}\phi_i)^2 \sum_{i=1}^{N+1} l_i^m\phi_i,\phi_j\right\rangle - \left\langle 6\sum_{i=1}^{N+1} k_i^{m-1}\phi_i \sum_{i=1}^{N+1} k_i^{m-2}\phi_i \sum_{i=1}^{N+1} l_i^m\phi_i,\phi_j\right\rangle\right. \\
&+\left\langle (\sum_{i=1}^{N+1} k_i^{m-2}\phi_i)^2 \sum_{i=1}^{N+1} l_i^m\phi_i,\phi_j\right\rangle + \left\langle 9(\sum_{i=1}^{N+1} k_i^{m-1}\phi_i)^2 \sum_{i=1}^{N+1} l_i^{m-1}\phi_i,\phi_j\right\rangle \\
&\left.-\left\langle 6\sum_{i=1}^{N+1} k_i^{m-1}\phi_i \sum_{i=1}^{N+1} k_i^{m-2}\phi_i \sum_{i=1}^{N+1} l_i^{m-1}\phi_i,\phi_j\right\rangle + \left\langle (\sum_{i=1}^{N+1} k_i^{m-2}\phi_i)^2 \sum_{i=1}^{N+1} l_i^{m-1}\phi_i,\phi_j\right\rangle\right), \qquad (3.30)\\
&\text{for } j = 1,2,\ldots,N+1 \quad , m = 3,4,\ldots,M+1\,.
\end{aligned}
$$

We next define the following matrices and vectors

$$
\begin{aligned}
&[A]_{i,j} = \mathcal{A}(\phi_i,\phi_j), \quad [M]_{i,j} = \langle \phi_i,\phi_j\rangle\,, \quad [Q_1^m]_{i,j} = \left\langle \phi_i(\sum_{r=1}^{N+1} k_r^{m-1}\phi_r \sum_{s=1}^{N+1} k_s^{m-1}\phi_s),\phi_j\right\rangle\,,\\
&[Q_2^m]_{i,j} = \left\langle \phi_i(\sum_{r=1}^{N+1} k_r^{m-1}\phi_r \sum_{s=1}^{N+1} k_s^{m-2}\phi_s),\phi_j\right\rangle, \quad [Q_3^m]_{i,j} = \left\langle \phi_i(\sum_{r=1}^{N+1} k_r^{m-2}\phi_r \sum_{s=1}^{N+1} k_s^{m-2}\phi_s),\phi_j\right\rangle\,,\\
&\mathbf{k^m} = [k_1^m \quad k_2^m \quad \ldots \quad k_{N+1}^m]^T, \quad \mathbf{l^m} = [l_1^m \quad l_2^m \quad \ldots \quad l_{N+1}^m]^T\,,\\
&\mathbf{z_1} = [\langle a,\phi_1\rangle \quad \langle a,\phi_2\rangle \quad \ldots \langle a,\phi_{N+1}\rangle]^T, \quad \mathbf{z_2} = [\langle b,\phi_1\rangle \quad \langle b,\phi_2\rangle \quad \ldots \langle b,\phi_{N+1}\rangle]^T\,.
\end{aligned}
$$

These matrix and vector definitions allow equations (3.29) and (3.30) to be written as

$$\left[\left(1+\frac{\gamma\triangle t}{2}\right)M+\frac{\triangle t}{2}A\right]\mathbf{k^m}=\left[\left(1-\frac{\gamma\triangle t}{2}\right)M-\frac{\triangle t}{2}A\right]\mathbf{k^{m-1}}$$
$$+\frac{\gamma\triangle t}{8}\left[9Q_1-6Q_2+Q_3\right]\mathbf{l^m}+\frac{\gamma\triangle t}{8}\left[9Q_1-6Q_2+Q_3\right]\mathbf{l^{m-1}}$$
$$+(\gamma\triangle t)\mathbf{z_1}\,, \tag{3.31}$$
$$\left[M+\frac{d\triangle t}{2}A+\frac{\gamma\triangle t}{8}\left(9Q_1-6Q_2+Q_3\right)\right]\mathbf{l^m}=\left[M-\frac{d\triangle t}{2}A\right]\mathbf{l^{m-1}}$$
$$-\frac{\gamma\triangle t}{8}\left[9Q_1-6Q_2+Q_3\right]\mathbf{l^{m-1}}+(\gamma\triangle t)\mathbf{z_2}\,, \tag{3.32}$$
$$\text{for}\, m\in\{3,4,\ldots,M+1\}\,.$$

Equations (3.31) and (3.32) constitute a linear system for the unknown vectors $\mathbf{k^m}$ and $\mathbf{l^m}$. Solving for these vectors allows us to approximate u and v in the $\mathcal{V}_h$ space for t_m, $m\in\{3,4,\ldots,M+1\}$. One further set of equations is required for the algorithm to numerically simulate using the Crank-Nicolson discretization, namely the predictor-corrector equations for t_2.

For the predictor-corrector scheme we denote $X^2\in\mathcal{V}_h$, $Y^2\in\mathcal{V}_h$ as

$$X^2=\sum_{i=1}^{N+1}e_i^2\phi_i\,,\, Y^2=\sum_{i=1}^{N+1}f_i^2\phi_i\,.$$

We also define the following additional matrices and vectors

$$[Q_4]_{i,j}=\left\langle\phi_i(\sum_{r=1}^{N+1}k_r^1\phi_r\sum_{s=1}^{N+1}k_s^1\phi_s),\phi_j\right\rangle,\quad [Q_5]_{i,j}=\left\langle\phi_i(\sum_{r=1}^{N+1}k_r^1\phi_r\sum_{s=1}^{N+1}e_s^2\phi_s),\phi_j\right\rangle,$$
$$[Q_6]_{i,j}=\left\langle\phi_i(\sum_{r=1}^{N+1}e_r^2\phi_r\sum_{s=1}^{N+1}e_s^2\phi_s),\phi_j\right\rangle,$$
$$\mathbf{e^2}=[e_1^2\quad e_2^2\quad\ldots\quad e_{N+1}^2]^T,\quad \mathbf{f^2}=[f_1^2\quad f_2^2\quad\ldots\quad f_{N+1}^2]^T\,.$$

Using these matrix and vector definitions, we can then write the predictor-corrector systems (3.27) and (3.28) as

$$\left(M+\frac{\triangle t}{2}A\right)\mathbf{e^2}=\left[(1-\gamma\triangle t)\,M-\frac{\triangle t}{2}A\right]\mathbf{k^1}+\gamma\triangle t\mathbf{z_1}+\gamma\triangle tQ_4\mathbf{l^1}\,, \tag{3.33}$$

$$\left(M+\frac{d\triangle t}{2}A\right)\mathbf{f^2}=\left[M-\frac{d\triangle t}{2}A\right]\mathbf{l^1}+\gamma\triangle t\mathbf{z_2}-\gamma\triangle tQ_4\mathbf{l^1}\,, \tag{3.34}$$

$$\left(M+\frac{\triangle t}{2}A\right)\mathbf{k^2}=\left[\left(1-\frac{\gamma\triangle t}{2}\right)M-\frac{\triangle t}{2}A\right]\mathbf{k^1}+\gamma\triangle t\mathbf{z_1}$$
$$-\frac{\gamma\triangle t}{2}M\mathbf{e^2}+\frac{\gamma\triangle t}{8}\left\{[Q_4+2Q_5+Q_6]\,\mathbf{f^2}+[Q_4+2Q_5+Q_6]\,\mathbf{l^1}\right\}\,, \tag{3.35}$$

$$\left(M+\frac{d\triangle t}{2}A\right)\mathbf{l^2}=\left[M-\frac{d\triangle t}{2}A\right]\mathbf{l^1}+\gamma\triangle t\mathbf{z_2}-$$
$$-\frac{\gamma\triangle t}{8}\left\{[Q_4+2Q_5+Q_6]\,\mathbf{f^2}+[Q_4+2Q_5+Q_6]\,\mathbf{l^1}\right\}\,. \tag{3.36}$$

Equations (3.33) and (3.34) are solved for vectors $\mathbf{e^2},\mathbf{f^2}$. With these coefficients we then solve equations (3.35) and (3.36) for U^2, V^2 via coefficient vectors $\mathbf{k^2},\mathbf{l^2}$.

Matrices A and M are typical for finite element methods, as seen in the Backward Euler section presented earlier in this chapter. The Q matrices are not standard in FEM. For their derivation we denote coefficients in various equations as a_i, b_i, $i\in\{1,\ldots,N+1\}$. Entries of the Q matrix can be derived as

$$[Q_{general}]_{i,i}=\int_{x_{i-1}}^{x_i}(\phi_i)^2(a_{i-1}\phi_{i-1}+a_i\phi_i)(b_{i-1}\phi_{i-1}+b_i\phi_i)$$
$$+\int_{x_i}^{x_{i+1}}(\phi_i)^2(a_i\phi_i+a_{i+1}\phi_{i+1})(b_i\phi_i+b_{i+1}\phi_{i+1}),\ i\in\{2,3,\ldots,N\}\,,$$
$$[Q_{general}]_{i,i-1}=\int_{x_{i-1}}^{x_i}(\phi_i)(\phi_{i-1})(a_{i-1}\phi_{i-1}+a_i\phi_i)(b_{i-1}\phi_{i-1}+b_i\phi_i),\ i\in\{2,3,\ldots,N\}\,,$$
$$[Q_{general}]_{i,i+1}=\int_{x_i}^{x_{i+1}}(\phi_i)(\phi_{i+1})(a_i\phi_i+a_{i+1}\phi_{i+1})(b_i\phi_i+b_{i+1}\phi_{i+1}),\ i\in\{2,3,\ldots,N\}\,,$$
$$[Q_{general}]_{1,1}=\int_{x_1}^{x_2}(\phi_1)^2(a_1\phi_1+a_2\phi_2)(b_1\phi_1+b_2\phi_2)\,,$$
$$[Q_{general}]_{1,2}=\int_{x_1}^{x_2}(\phi_1)(\phi_2)(a_1\phi_1+a_2\phi_2)(b_1\phi_1+b_2\phi_2)\,,$$
$$[Q_{general}]_{N+1,N}=\int_{x_N}^{x_{N+1}}(\phi_N)(\phi_{N+1})(a_N\phi_N+a_{N+1}\phi_{N+1})(b_N\phi_N+b_{N+1}\phi_{N+1})\,,$$
$$[Q_{general}]_{N+1,N+1}=\int_{x_N}^{x_{N+1}}(\phi_{N+1})^2(a_N\phi_N+a_{N+1}\phi_{N+1})(b_N\phi_N+b_{N+1}\phi_{N+1})\,.$$

These integrals when computed in Mathematica yield:

$$
\begin{aligned}
[Q_{general}]_{1,1} &= \frac{h_1}{60}(3a_1(4b_1+b_2)+a_2(3b_1+2b_2))\,,\\
[Q_{general}]_{1,2} &= \frac{h_1}{60}(a_1(3b_1+2b_2)+a_2(2b_1+3b_2))\,,\\
[Q_{general}]_{i,i-1} &= \frac{h_{i-1}}{60}(a_{i-1}(3b_{i-1}+2b_i)+a_i(2b_{i-1}+3b_i))\,,\\
[Q_{general}]_{i,i} &= \frac{h_{i-1}}{60}(a_{i-1}(2b_{i-1}+3b_i))+\frac{h_i}{60}(a_{i+1}(3b_i+2b_{i+1}))\\
&+\frac{3a_i}{60}(h_{i-1}b_{i-1}+4(h_{i-1}+h_i)b_i+h_ib_{i+1})\,,\\
[Q_{general}]_{i,i+1} &= \frac{h_i}{60}(a_i(3b_i+2b_{i+1})+a_{i+1}(2b_i+3b_{i+1}))\,,\\
[Q_{general}]_{N+1,N} &= \frac{h_N}{60}(a_N(3b_N+2b_{N+1})+a_{N+1}(2b_N+3b_{N+1}))\,,\\
[Q_{general}]_{N+1,N+1} &= \frac{h_N}{60}(a_N(2b_N+3b_{N+1})+3a_{N+1}(b_N+4b_{N+1}))\,.
\end{aligned}
$$

We note that for several of the Q matrices in this Crank-Nicolson Section, $a_i = b_i$ which yields further simplifications. For these Q matrices with a single type of coefficient, the integrals simplify to

$$
\begin{aligned}
[Q]_{1,1} &= \frac{h_1}{30}(6a_1^2+3a_1a_2+a_2^2))\,,\\
[Q]_{1,2} &= \frac{h_1}{60}(3a_1^2+4a_1a_2+3a_2^2))\,,\\
[Q]_{i,i-1} &= \frac{h_{i-1}}{60}(3a_{i-1}^2+4a_{i-1}a_i+3a_i^2)\,,\\
[Q]_{i,i} &= \frac{h_{i-1}}{30}(a_{i-1}^2+3a_{i-1}a_i))+\frac{h_i}{30}(a_{i+1}^2+3a_ia_{i+1}))+\frac{(h_{i-1}+h_i)}{30}(6a_i^2)\,,\\
[Q]_{i,i+1} &= \frac{h_i}{60}(3a_i^2+4a_ia_{i+1}+3a_{i+1}^2)\,,\\
[Q]_{N+1,N} &= \frac{h_N}{60}(3a_N^2+4a_Na_{N+1}+3a_{N+1}^2)\,,\\
[Q]_{N+1,N+1} &= \frac{h_N}{30}(a_N^2+3a_Na_{N+1}+6a_{N+1}^2)\,.
\end{aligned}
$$

The algorithm from the Backward Euler section was modified to also solve equations (3.31) and (3.32). Specifically, this algorithm uses input from a user to select the discretization to use. Examples of this algorithm's patterns can be found later in this chapter.

3.3 Finite Element Method: Gierer-Meinhardt Kinetics

In this section we describe a finite element method using both Backward Euler and Crank-Nicolson discretizations for the second set of benchmark reaction kinetics. Specifically, we deal with

the variational formulation with Gierer-Meinhardt reaction kinetics in this section. The variational formulation of interest is

$$\int_\alpha^\beta \frac{\partial u}{\partial t} w + \int_\alpha^\beta \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = \int_\alpha^\beta \gamma \left(a - bu + \frac{u^2}{v(1+\kappa u^2)} \right) w, \quad \forall w \in \mathcal{V}\,, \tag{3.37}$$

$$\int_\alpha^\beta \frac{\partial v}{\partial t} w + d\int_\alpha^\beta \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = \int_\alpha^\beta \gamma(u^2 - v)w, \quad \forall w \in \mathcal{V}\,. \tag{3.38}$$

For these kinetics, we use the spatial and temporal meshes defined in the Schnakenberg FEM, along with the spaces $\mathcal{V}$, $\mathcal{V}_h$.

3.3.1 Backward Euler Finite Element Method

A Backward Euler finite element method is found for equations (3.37) and (3.38) by first discretizing with a Backward Euler scheme as seen in Section 3.2.1 . We thus obtain for equations (3.37) and (3.38),

$$\left\langle \frac{U^m - U^{m-1}}{\triangle t}, w \right\rangle + \mathcal{A}(U^m, w) = \left\langle \gamma(a - bU^m + \frac{(U^m)^2}{V^m(1+\kappa(U^m)^2)}), w \right\rangle\,, \tag{3.39}$$

$$\left\langle \frac{V^m - V^{m-1}}{\triangle t}, w \right\rangle + d\mathcal{A}(V^m, w) = \left\langle \gamma((U^m)^2 - V^m), w \right\rangle\,, \tag{3.40}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for } m \in \{2, 3, \ldots, M+1\}\,.$$

We also approximate the given initial value data g_1, g_2 respectively by U^1, $V^1 \in \mathcal{V}_h$. Simplification of equations (3.39) and (3.40) is conducted using the bilinearity of the $<\cdot,\cdot>$ and $\mathcal{A}$ operations along with linearization of the $(U^m)^2$ terms. We follow the same linearization as used in the Schnakenberg kinetics section, namely $(U^m)^2 \approx (U^{m-1})^2$. Linearization and grouping thus yields

$$(1 + b\gamma\triangle t)\left\langle U^m, w\right\rangle + \triangle t\mathcal{A}(U^m, w) = \left\langle U^{m-1}, w\right\rangle + \gamma\triangle t\left\langle a, w\right\rangle + \gamma\triangle t\left\langle \frac{\left(U^{m-1}\right)^2}{V^m(1+\kappa(U^{m-1})^2)}), w \right\rangle\,, \tag{3.41}$$

$$(1 + \gamma\triangle t)\left\langle V^m, w\right\rangle + d\triangle t\mathcal{A}(V^m, w) = \left\langle V^{m-1}, w\right\rangle + \gamma\triangle t\left\langle (U^{m-1})^2, w\right\rangle\,, \tag{3.42}$$

$$\forall w \in \mathcal{V}_h, \quad \text{for } m \in \{2, 3, \ldots, M+1\}\,.$$

Next, we use the basis functions of the $\mathcal{V}_h$ space, to write for terms of $U^m\,, V^m$:

$$U^m = \sum_{i=1}^{N+1} k_i^m \phi_i,\ k_i^m \in \mathbb{R}, \quad V^m = \sum_{i=1}^{N+1} l_i^m \phi_i,\ l_i^m \in \mathbb{R}\,.$$

Using these linear combinations of basis functions in equations (3.41) and (3.42), while noting that

these equations hold for all $w \in \mathcal{V}_h$, and therefore for any ϕ_j, $j \in \{1, \ldots, N+1\}$ yields

$$(1 + b\gamma\triangle t) \sum_{i=1}^{N+1} k_i^m \langle \phi_i, \phi_j \rangle + \triangle t \sum_{i=1}^{N+1} k_i^m \mathcal{A}(\phi_i, \phi_j) = \sum_{i=1}^{N+1} k_i^{m-1} \langle \phi_i, \phi_j \rangle$$
$$+ \gamma\triangle t \langle a, \phi_j \rangle + \gamma\triangle t \langle \star_2^m, \phi_j \rangle \ , \tag{3.43}$$
$$(1 + \gamma\triangle t) \sum_{i=1}^{N+1} l_i^m \langle \phi_i, \phi_j \rangle + d\triangle t \sum_{i=1}^{N+1} l_i^m \mathcal{A}(\phi_i, \phi_j) = \sum_{i=1}^{N+1} l_i^{m-1} \langle \phi_i, \phi_j \rangle$$
$$+ \gamma\triangle t \langle \star^m, \phi_j \rangle \ , \tag{3.44}$$
$$\text{for } m \in \{2, 3, \ldots, N+1\},\ j \in \{1, 2, \ldots, N+1\}\,.$$

Where in equations (3.43) and (3.44) we have denoted

$$\star^m = \left(\sum_{i=1}^{N+1} k_i^{m-1} \phi_i \right)^2 , \quad \star_2^m = \frac{\star^m}{\left(\sum_{i=1}^{N+1} l_i^m \phi_i \right) (1 + \kappa \star^m)} \,.$$

We now define the following matrices and vectors

$$[A]_{i,j} = \mathcal{A}(\phi_i, \phi_j), \quad [M]_{i,j} = \langle \phi_i, \phi_j \rangle \ ,$$
$$\mathbf{k^m} = [k_1^m \quad k_2^m \quad \ldots \quad k_{N+1}^m]^T, \quad \mathbf{l^m} = [l_1^m \quad l_2^m \quad \ldots \quad l_{N+1}^m]^T \,,$$
$$\mathbf{q^m} = [\langle \star^m, \phi_1 \rangle \quad \langle \star^m, \phi_2 \rangle \quad \ldots \langle \star^m, \phi_{N+1} \rangle]^T \ ,$$
$$\mathbf{q_2^m} = [\langle \star_2^m, \phi_1 \rangle \quad \langle \star_2^m, \phi_2 \rangle \quad \ldots \langle \star_2^m, \phi_{N+1} \rangle]^T \ ,$$
$$\mathbf{z} = [\langle a, \phi_1 \rangle \quad \langle a, \phi_2 \rangle \quad \ldots \langle a, \phi_{N+1} \rangle]^T \,.$$

Using these matrices and vectors we can write equations (3.43) and (3.44) as

$$[(1 + b\gamma\triangle t)M + \triangle t A]\, \mathbf{k^m} = M\mathbf{k^{m-1}} + (\gamma\triangle t)(\mathbf{z} + \mathbf{q_2^m}) \,, \tag{3.45}$$
$$[(1 + \gamma\triangle t)M + d\triangle t A]\, \mathbf{l^m} = M\mathbf{l^{m-1}} + (\gamma\triangle t)\mathbf{q^m} \,, \tag{3.46}$$
$$\text{for } m = 2, 3, \ldots, N+1 \,.$$

Equations (3.45) and (3.46) define a linear system for the unknown vectors $\mathbf{k^m}, \mathbf{l^m}$. As in the Schnakenberg case, matrices A, M are standard. The entries of vectors $\mathbf{q^m}, \mathbf{q_2^m}$ are computed numerically at each time step. For example, at t_2 we find the i^{th} entries, $i \in \{2, 3, \ldots, N\}$, of $\mathbf{q^2}$, and $\mathbf{q_2^2}$ as

$$\left[\mathbf{q^2}\right]_i = \int_{x_{i-1}}^{x_{i+1}} \left(\sum_{i=1}^{N+1} k_i^1 \phi_i\right)^2 \phi_i \, dx \,,$$

$$\left[\mathbf{q_2^2}\right]_i = \int_{x_{i-1}}^{x_{i+1}} \frac{\left(\sum_{i=1}^{N+1} k_i^1 \phi_i\right)^2}{\left(\sum_{i=1}^{N+1} l_i^2 \phi_i\right)\left(1 + \kappa\left(\sum_{i=1}^{N+1} k_i^1 \phi_i\right)^2\right)} \phi_i \, dx \,.$$

These integrals are not analytically computed, but rather are numerically approximated at each time step. The linear system of equations (3.45) and (3.46) were added to the algorithm for Schnakenberg kinetics, such that the algorithm asks for user input to which reaction kinetics are to be modeled. Examples of the patterns produced by the algorithm are presented later in the chapter.

3.3.2 Crank-Nicolson Finite Element Method

A Crank-Nicolson finite element method for equations (3.37) and (3.38) is given by the system

$$\left\langle \frac{U^m - U^{m-1}}{\triangle t}, w \right\rangle + \mathcal{A}(U^{m-1/2}, w) = \left\langle \gamma(a - bU^{m-1/2} + \frac{\left(U^{m-1/2}\right)^2}{V^{m-1/2}(1 + \kappa(U^{m-1/2})^2)}), w \right\rangle, \quad (3.47)$$

$$\left\langle \frac{V^m - V^{m-1}}{\triangle t}, w \right\rangle + d\mathcal{A}(V^{m-1/2}, w) = \left\langle \gamma((U^{m-1/2})^2 - V^{m-1/2}), w \right\rangle, \quad (3.48)$$

$\forall w \in \mathcal{V}_h$, $m \in \{2, 3, \ldots, M+1\}$.

We also approximate the given initial value data g_1, g_2 respectively by U^1, $V^1 \in \mathcal{V}_h$. Simplification of equations (3.47) and (3.48) is conducted by using the bilinearity of the $< \cdot, \cdot >, \mathcal{A}$ operators, along with the linearization of $(U^{m-1/2})^2$ noted in Section 3.2.2 . Namely, the linearization is given by

$$(U^{m-1/2})^2 \approx \left(\frac{3U^{m-1} - U^{m-2}}{2}\right)^2 .$$

We thus write equations (3.47) and (3.48) as

$$\left\langle U^m - U^{m-1}, w \right\rangle + \frac{\triangle t}{2}\mathcal{A}\left(U^m + U^{m-1}, w\right) = \gamma \triangle t \left\langle a, w \right\rangle - \frac{b\gamma \triangle t}{2}\left\langle U^m + U^{m-1}, w \right\rangle$$
$$+ 2\gamma \triangle t \left\langle \frac{(3U^{m-1} - U^{m-2})^2}{(V^m + V^{m-1})(4 + \kappa(3U^{m-1} - U^{m-2})^2}, w \right\rangle, \quad (3.49)$$

$$\langle V^m - V^{m-1}, w\rangle + \frac{d\triangle t}{2}\mathcal{A}\left(V^m + V^{m-1}, w\right) = \frac{\gamma\triangle t}{4}\left\langle (3U^m - U^{m-2})^2, w\right\rangle$$
$$- \frac{\gamma\triangle t}{2}\left\langle V^m + V^{m-1}, w\right\rangle , \tag{3.50}$$
$$\forall w \in \mathcal{V}_h,\, m \in \{3, 4, \ldots, M+1\}\,.$$

Equations (3.49) and (3.50) can be simplified further by grouping, which yields

$$\left(1 + \frac{b\gamma\triangle t}{2}\right)\langle U^m, w\rangle + \frac{\triangle t}{2}\mathcal{A}(U^m, w) = \left(1 - \frac{b\gamma\triangle t}{2}\right)\left\langle U^{m-1}, w\right\rangle$$
$$- \frac{\triangle t}{2}\mathcal{A}(U^{m-1}, w) + \gamma\triangle t\,\langle a, w\rangle + 2\gamma\triangle t\left\langle \frac{(3U^{m-1} - U^{m-2})^2}{(V^m + V^{m-1})(4 + \kappa(3U^{m-1} - U^{m-2})^2)}, w\right\rangle , \tag{3.51}$$
$$\left(1 + \frac{\gamma\triangle t}{2}\right)\langle V^m, w\rangle + \frac{d\triangle t}{2}\mathcal{A}(V^m, w) = \left(1 - \frac{\gamma\triangle t}{2}\right)\left\langle V^{m-1}, w\right\rangle$$
$$- \frac{d\triangle t}{2}\mathcal{A}(V^{m-1}, w) + \frac{\gamma\triangle t}{4}\left\langle (3U^{m-1} - U^{m-2})^2, w\right\rangle , \tag{3.52}$$
$$\forall w \in \mathcal{V}_h,\, m \in \{3, 4, \ldots, M+1\}\,.$$

Using the hat basis functions of the $\mathcal{V}_h$ space, we can write

$$U^m = \sum_{i=1}^{N+1} k_i^m \phi_i,\, k_i^m \in \mathbb{R}, \quad V^m = \sum_{i=1}^{N+1} l_i^m \phi_i,\, l_i^m \in \mathbb{R}\,.$$

Using these basis functions, and their compact support, to further expand equations (3.51) and (3.52) our system becomes

$$\left(1 + \frac{b\gamma\triangle t}{2}\right)\sum_{i=1}^{N+1} k_i^m < \phi_i, \phi_j > + \left(\frac{\triangle t}{2}\right)\sum_{i=1}^{N+1} k_i^m \mathcal{A}(\phi_i, \phi_j)$$
$$= \left(1 - \frac{b\gamma\triangle t}{2}\right)\sum_{i=1}^{N+1} k_i^{m-1} < \phi_i, \phi_j > - \left(\frac{\triangle t}{2}\right)\sum_{i=1}^{N+1} k_i^{m-1}\mathcal{A}(\phi_i, \phi_j)$$
$$+ (2\gamma\triangle t)\left\langle \frac{\star^m}{\star_2^m}, \phi_j\right\rangle + \gamma\triangle t < a, \phi_j > , \tag{3.53}$$
$$\left(1 + \frac{\gamma\triangle t}{2}\right)\sum_{i=1}^{N+1} l_i^m < \phi_i, \phi_j > + \left(\frac{d\triangle t}{2}\right)\sum_{i=1}^{N+1} l_i^m \mathcal{A}(\phi_i, \phi_j)$$
$$= \left(1 - \frac{\gamma\triangle t}{2}\right)\sum_{i=1}^{N+1} l_i^{m-1} < \phi_i, \phi_j > - \left(\frac{d\triangle t}{2}\right)\sum_{i=1}^{N+1} l_i^{m-1}\mathcal{A}(\phi_i, \phi_j)$$
$$+ \left(\frac{\gamma\triangle t}{4}\right) < \star^m, \phi_j > , \tag{3.54}$$
$$\text{for } j \in \{1, 2, \ldots, N+1\},\, m \in \{3, 4, \ldots, M+1\}\,.$$

Where for equations (3.53) and (3.54) we have denoted

$$\star^m = \left[\sum_{i=1}^{N+1} \left(3k_i^{m-1} - k_i^{m-2}\right)\phi_i\right]^2, \; \star_2^m = \left[\sum_{i=1}^{N+1} \left(l_i^m + l_i^{m-1}\right)\phi_i\right] * \left[4 + \kappa\star^m\right] .$$

We next define the following matrices and vectors

$$\begin{aligned}
&[A]_{i,j} = \mathcal{A}(\phi_i, \phi_j), \quad [M]_{i,j} = \langle \phi_i, \phi_j \rangle \, , \\
&\mathbf{k^m} = [k_1^m \quad k_2^m \quad \dots \quad k_{N+1}^m]^T, \quad \mathbf{l^m} = [l_1^m \quad l_2^m \quad \dots \quad l_{N+1}^m]^T , \\
&\mathbf{q^m} = \left[\left\langle \frac{\star^m}{\star_2^m}, \phi_1 \right\rangle \quad \left\langle \frac{\star^m}{\star_2^m}, \phi_2 \right\rangle \quad \dots \left\langle \frac{\star^m}{\star_2^m}, \phi_{N+1} \right\rangle\right]^T , \\
&\mathbf{q_2^m} = [\langle \star^m, \phi_1 \rangle \quad \langle \star^m, \phi_2 \rangle \quad \dots \langle \star^m, \phi_{N+1} \rangle]^T \, , \\
&\mathbf{z} = [\langle a, \phi_1 \rangle \quad \langle a, \phi_2 \rangle \quad \dots \langle a, \phi_{N+1} \rangle]^T .
\end{aligned}$$

Using these matrices and vectors allows equations (3.51) and (3.52) to be written as

$$\left[\left(1 + \frac{b\gamma\triangle t}{2}\right) M + \frac{\triangle t}{2} A\right] \mathbf{k^m} = \left[\left(1 - \frac{b\gamma\triangle t}{2}\right) M - \frac{\triangle t}{2} A\right] \mathbf{k^{m-1}} + 2\gamma\triangle t \mathbf{q^m} + \gamma\triangle t \mathbf{z} \, , \tag{3.55}$$

$$\left[\left(1 + \frac{\gamma\triangle t}{2}\right) M + \frac{d\triangle t}{2} A\right] \mathbf{l^m} = \left[\left(1 - \frac{\gamma\triangle t}{2}\right) M - \frac{d\triangle t}{2} A\right] \mathbf{l^{m-1}} + (\frac{\gamma\triangle t}{4}) \mathbf{q_2^m} \, , \tag{3.56}$$

for $m \in \{3, 4, \dots, M+1\}$.

Equations (3.55) and (3.56) constitute a linear system for the unknown vectors $\mathbf{k^m}$ and $\mathbf{l^m}$. Solving for these vectors allows us to approximate u and v in the space $\mathcal{V}_h$. We note that solutions are found by solving first for $\mathbf{l^m}$ and then for $\mathbf{k^m}$. This is due to the $\mathbf{q^m}$ vector used in solving $\mathbf{k^m}$ calling for current $\mathbf{l^m}$ entries. We also note that equations (3.55) and (3.56) require a separate scheme to solve for t_2. Consequently, we use a similar predictor-correcter scheme to that presented in Section 3.2.2 . We let $X^1 = U^1, Y^1 = V^1$, and then

$$\begin{aligned}
&\left\langle \frac{X^2 - X^1}{\triangle t}, w \right\rangle + \mathcal{A}\left(\frac{X^2 + X^1}{2}, w\right) = \left\langle \gamma(a - bX^1 + \frac{(X^1)^2}{Y^1(1 + \kappa(X^1)^2)}, w \right\rangle \, , \\
&\left\langle \frac{Y^2 - Y^1}{\triangle t}, w \right\rangle + \mathcal{A}\left(d\frac{Y^2 + Y^1}{2}, w\right) = \langle \gamma((X^1)^2 - Y^1), w \rangle \, , \qquad (3.57) \\
&\left\langle \frac{U^2 - U^1}{\triangle t}, w \right\rangle + \mathcal{A}\left(\frac{U^2 + U^1}{2}, w\right) = \left\langle \gamma(a - bX^{3/2} + \frac{(X^{3/2})^2}{Y^{3/2}(1 + \kappa(X^{3/2})^2)}, w \right\rangle \, , \\
&\left\langle \frac{V^2 - V^1}{\triangle t}, w \right\rangle + \mathcal{A}\left(d\frac{V^2 + V^1}{2}, w\right) = \left\langle \gamma((X^{3/2})^2 - Y^{3/2}), w \right\rangle \, , \qquad (3.58)
\end{aligned}$$

$\forall w \in \mathcal{V}_h$,

where $X^{3/2} = (X^2 + X^1)/2$, $Y^{3/2} = (Y^2 + Y^1)/2$.

Simplification of system (3.57), using the linearity of the operations, yields

$$\begin{aligned}
&\left\langle X^2, w\right\rangle + \frac{\triangle t}{2}\mathcal{A}\left(X^2, w\right) = (1 - b\gamma\triangle t)\left\langle X^1, w\right\rangle \\
&- \frac{\triangle t}{2}\mathcal{A}\left(X^1, w\right) + \gamma\triangle t\left\langle \frac{(X^1)^2}{Y^1(1+\kappa(X^1)^2)}, w\right\rangle + \gamma\triangle t\left\langle a, w\right\rangle , \\
&\left\langle Y^2, w\right\rangle + \frac{d\triangle t}{2}\mathcal{A}\left(Y^2, w\right) = (1 - \gamma\triangle t)\left\langle Y^1, w\right\rangle - \frac{d\triangle t}{2}\mathcal{A}\left(Y^1, w\right) + \gamma\triangle t\left\langle (X^1)^2, w\right\rangle . \qquad (3.59)
\end{aligned}$$

Similar simplification of system (3.58) yields

$$\begin{aligned}
&\left\langle U^2, w\right\rangle + \frac{\triangle t}{2}\mathcal{A}\left(U^2, w\right) = \frac{-b\gamma\triangle t}{2}\left\langle X^2, w\right\rangle + \left(1 - \frac{b\gamma\triangle t}{2}\right)\left\langle X^1, w\right\rangle \\
&+ \gamma\triangle t\left\langle a, w\right\rangle - \frac{\triangle t}{2}\mathcal{A}(X^1, w) + 2\gamma\triangle t\left\langle \frac{(X^1 + X^2)^2}{(Y^1 + Y^2)(4 + \kappa(X^1 + X^2)^2)}\right\rangle , \\
&\left\langle V^2, w\right\rangle + \frac{d\triangle t}{2}\mathcal{A}\left(V^2, w\right) = \left(1 - \frac{\gamma\triangle t}{2}\right)\left\langle Y^1, w\right\rangle - \frac{d\triangle t}{2}\mathcal{A}(Y^1, w) \\
&- \frac{\gamma\triangle t}{2}\left\langle Y^2, w\right\rangle + \frac{\gamma\triangle t}{4}\left\langle (X^1 + X^2)^2, w\right\rangle . \qquad (3.60)
\end{aligned}$$

Using basis functions of $\mathcal{V}_h$ we can write

$$\begin{aligned}
&X^2 = \sum_{i=1}^{N+1} e_i^2\phi_i,\ Y^2 = \sum_{i=1}^{N+1} f_i^2\phi_i,\ X^1 = U^1 = \sum_{i=1}^{N+1} k_i^1\phi_i, \\
&Y^1 = V^1 = \sum_{i=1}^{N+1} l_i^1\phi_i,\ U^2 = \sum_{i=1}^{N+1} k_i^2\phi_i,\ V^2 = \sum_{i=1}^{N+1} l_i^2\phi_i .
\end{aligned}$$

These linear combinations of basis functions, while restricting w to $\phi_j,\ j = 1, 2, \ldots, N+1$ allows systems (3.59) and (3.60) to be written respectively as

$$\begin{aligned}
&\sum_{i=1}^{N+1} e_i^2\left[< \phi_i, \phi_j > + \frac{\triangle t}{2}\mathcal{A}(\phi_i, \phi_j)\right] = \gamma\triangle t < a, \phi_j > \\
&+ \sum_{i=1}^{N+1} k_i^1\left[(1 - b\gamma\triangle t) < \phi_i, \phi_j > - \frac{\triangle t}{2}\mathcal{A}(\phi_i, \phi_j)\right] + (\gamma\triangle t)\left\langle \frac{\star_3}{\star_4}, \phi_j\right\rangle , \\
&\sum_{i=1}^{N+1} f_i^2\left[< \phi_i, \phi_j > + \frac{d\triangle t}{2}\mathcal{A}(\phi_i, \phi_j)\right] = \sum_{i=1}^{N+1} l_i^1\left[(1 - \gamma\triangle t) < \phi_i, \phi_j > \right. \\
&\left. - \frac{d\triangle t}{2}\mathcal{A}(\phi_i, \phi_j)\right] + \gamma\triangle t\left\langle \star_3, \phi_j\right\rangle , \qquad (3.61)
\end{aligned}$$

$$\sum_{i=1}^{N+1} k_i^2 \left[< \phi_i, \phi_j > + \frac{\triangle t}{2} \mathcal{A}(\phi_i, \phi_j) \right] = \gamma \triangle t < a, \phi_j >$$
$$+ \sum_{i=1}^{N+1} k_i^1 \left[\left(1 - \frac{b\gamma \triangle t}{2} \right) < \phi_i, \phi_j > - \frac{\triangle t}{2} \mathcal{A}(\phi_i, \phi_j) \right]$$
$$+ \sum_{i=1}^{N+1} e_i^2 \left[\left(\frac{-b\gamma \triangle t}{2} \right) < \phi_i, \phi_j > \right] + 2\gamma \triangle t \left\langle \frac{\star_5}{\star_6}, \phi_j \right\rangle ,$$
$$\sum_{i=1}^{N+1} l_i^2 \left[< \phi_i, \phi_j > + \frac{d \triangle t}{2} \mathcal{A}(\phi_i, \phi_j) \right] = \sum_{i=1}^{N+1} l_i^1 \left[(1 - \frac{\gamma \triangle t}{2}) < \phi_i, \phi_j > - \frac{d \triangle t}{2} \mathcal{A}(\phi_i, \phi_j) \right]$$
$$+ \sum_{i=1}^{N+1} f_i^2 \left[\frac{-\gamma \triangle t}{2} \left\langle \phi_i, \phi_j \right\rangle \right] + \frac{\gamma \triangle t}{4} \left\langle \star_5, \phi_j \right\rangle , \tag{3.62}$$
$$\text{for } j \in \{1, 2, \ldots, N+1\} .$$

In equations (3.61) and (3.62) we have used the notations

$$\star_3 = \left(\sum_{i=1}^{N+1} k_i^1 \phi_i \right)^2 , \star_4 = \left(\sum_{i=1}^{N+1} l_i^1 \phi_i \right) (1 + \kappa \star_3) ,$$
$$\star_5 = \left[\sum_{i=1}^{N+1} \left(k_i^1 + e_i^2 \right) \phi_i \right]^2 , \star_6 = \left[\sum_{i=1}^{N+1} \left(l_i^1 + f_i^2 \right) \phi_i \right] * \left[4 + \kappa \star_5 \right] .$$

We next define the additional matrices and vectors

$$\mathbf{e^2} = [e_1^2 \quad e_2^2 \quad \ldots \quad e_{N+1}^2]^T, \quad \mathbf{f^2} = [f_1^2 \quad f_2^2 \quad \ldots \quad f_{N+1}^2]^T ,$$
$$\mathbf{q_3} = \left[\left\langle \frac{\star_3}{\star_4}, \phi_1 \right\rangle \quad \left\langle \frac{\star_3}{\star_4}, \phi_2 \right\rangle \quad \ldots \left\langle \frac{\star_3}{\star_4}, \phi_{N+1} \right\rangle \right]^T ,$$
$$\mathbf{q_4} = \left[\langle \star_3, \phi_1 \rangle \quad \langle \star_3, \phi_2 \rangle \quad \ldots \langle \star_3, \phi_{N+1} \rangle \right]^T ,$$
$$\mathbf{q_5} = \left[\left\langle \frac{\star_5}{\star_6}, \phi_1 \right\rangle \quad \left\langle \frac{\star_5}{\star_6}, \phi_2 \right\rangle \quad \ldots \left\langle \frac{\star_5}{\star_6}, \phi_{N+1} \right\rangle \right]^T ,$$
$$\mathbf{q_6} = \left[\langle \star_5, \phi_1 \rangle \quad \langle \star_5, \phi_2 \rangle \quad \ldots \langle \star_5, \phi_{N+1} \rangle \right]^T .$$

Thus, we write systems (3.61) and (3.62) as:

$$\left[M+\frac{\triangle t}{2}A\right]\mathbf{e^2}=\left[(1-b\gamma\triangle t)\,M-\frac{\triangle t}{2}A\right]\mathbf{k^1}+\gamma\triangle t\mathbf{q}_3+\gamma\triangle t\mathbf{z}\,, \tag{3.63}$$

$$\left[M+\frac{d\triangle t}{2}A\right]\mathbf{f^2}=\left[(1-\gamma\triangle t)\,M-\frac{d\triangle t}{2}A\right]\mathbf{l^1}+\gamma\triangle t\mathbf{q_4}\,, \tag{3.64}$$

$$\begin{aligned}\left[M+\frac{\triangle t}{2}A\right]\mathbf{k^2}&=\left[\left(1-\frac{b\gamma\triangle t}{2}\right)M-\frac{\triangle t}{2}A\right]\mathbf{k^1}\\&+\left[\frac{-b\gamma\triangle t}{2}M\right]\mathbf{e^2}+2\gamma\triangle t\mathbf{q}_5+\gamma\triangle t\mathbf{z}\,,\end{aligned} \tag{3.65}$$

$$\begin{aligned}\left[M+\frac{d\triangle t}{2}A\right]\mathbf{l^2}&=\left[\left(1-\frac{\gamma\triangle t}{2}\right)M-\frac{d\triangle t}{2}A\right]\mathbf{l^1}\\&+\left[\frac{-\gamma\triangle t}{2}M\right]\mathbf{f^2}+\frac{\gamma\triangle t}{4}\mathbf{q_6}\,.\end{aligned} \tag{3.66}$$

Equations (3.63) and (3.64) constitute a linear system for the unknowns $e_i^2,\ f_i^2,\ i\in\{1,\ldots,N+1\}$. Similarly, equations (3.65) and (3.66) constitute a linear system for the unknowns $k_i^2,\ l_i^2,\ i\in\{1,\ldots,N+1\}$ that when solved give the approximations $U^2,\ V^2\in\mathcal{V}_h$.

In the next section we present results of an algorithm that models pattern formation on a fixed spatial domain. This algorithm uses equations (3.53) and (3.54) for Gierer-Meinhardt kinetics with Crank-Nicolson discretization.

3.4 Computational Results

In this section we present the patterns modeled by an algorithm that utilizes the linear systems presented in Sections 3.2.1-3.3.2 . Two versions of initial conditions are presented for the algorithm. Validation of this algorithm is conducted by studying mode isolation of patterns as presented in Sections 2.4.1 and 2.4.2 . The patterns produced are also compared to those found in literature [11]. Finally, we discuss the convergence of the algorithm for the two choices of discretization and linearization.

3.4.1 Initial Conditions

For this model we have used two sets of initial conditions (ICs). The two sets of ICs differ in one regard: the first set of ICs uses random perturbations, while the second set's perturbations are not random. Let us explicitly describe the two sets of ICs used in this algorithm. Let u_s, v_s denote the homogeneous steady state of the reaction kinetics of Sections 2.4.1 and 2.4.2 . The first set of ICs is given by

$$\mathbf{g}(x)=\begin{bmatrix} g_1(x)\\ g_2(x)\end{bmatrix}=\begin{bmatrix} u_s+\epsilon\sum_k r_{(1,k)}\cos(k\pi x)\\ v_s+\epsilon\sum_k r_{(2,k)}\cos(k\pi x)\end{bmatrix}. \tag{3.67}$$

For equation (3.67) $r_{(1,k)}$, $r_{(2,k)}$ are pseudo-random numbers in $(0,1)$ for each k. We also take $k = 39$ for this specific IC, but any sufficiently large integer will work. We also take use scaling parameter $\epsilon = 0.001$ for this IC.

The second set of IC's is given by

$$\mathbf{g}(x) = \begin{bmatrix} g_1(x) \\ g_2(x) \end{bmatrix} = \begin{bmatrix} u_s + \epsilon \sum_k \cos(k\pi x) \\ v_s + \epsilon \sum_k \cos(k\pi x) \end{bmatrix}, \tag{3.68}$$

where we again take $k = 39$, $\epsilon = 0.001$. For the majority of patterns produced by our algorithm we have used the second set of ICs, equation (3.68). We have used this choice of ICs because random perturbations can cause the patterns produced to be phase shifted. This phase shifting makes it difficult to approximate error and convergence, and consequently we use non-random ICs.

3.4.2 Schnakenberg Results

Our algorithm produces patterns for Schnakenberg kinetics using both Backward Euler and Crank-Nicolson discretizations. Figure 3.1 shows a surface plot of the approximation U to illustrate pattern formation with Schnakenberg kinetics.

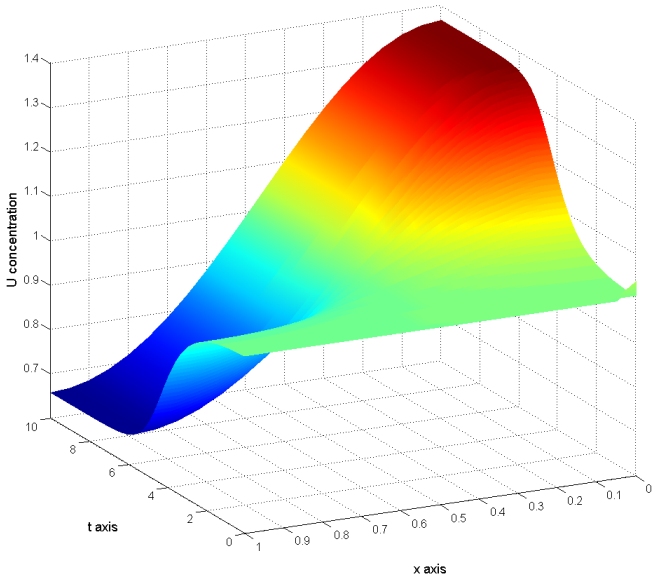
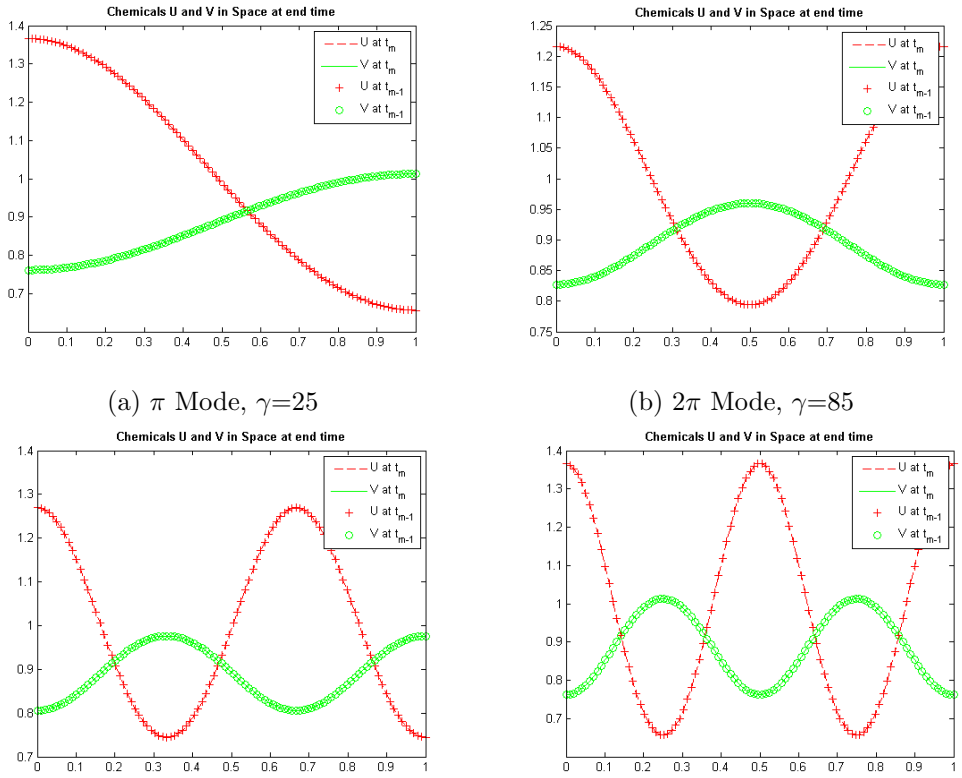


Figure 3.1: Schnakenberg Pattern Formation

We first discuss mode isolation of the patterns to validate the algorithm. Mode isolation is conducted by fixing parameters a, b, d and using a value for γ such that only a certain wavelength of pattern should be excited. Figure 3.2 shows the patterns produced by these mode isolation tests for the Backward Euler FEM. Mode isolation tests were also conducted using the Crank-Nicolson

discretization. Figure 3.3 illustrates the Crank-Nicolson mode isolation tests.



(a) π Mode, γ=25

(b) 2π Mode, γ=85

(c) 3π Mode, γ=200

(d) 4π Mode, γ=400

Figure 3.2: Backward Euler FEM on a fixed domain and with Schnakenberg kinetics. Mode isolation tests with parameters: $a = 0.1, b = 0.9, d = 10$.

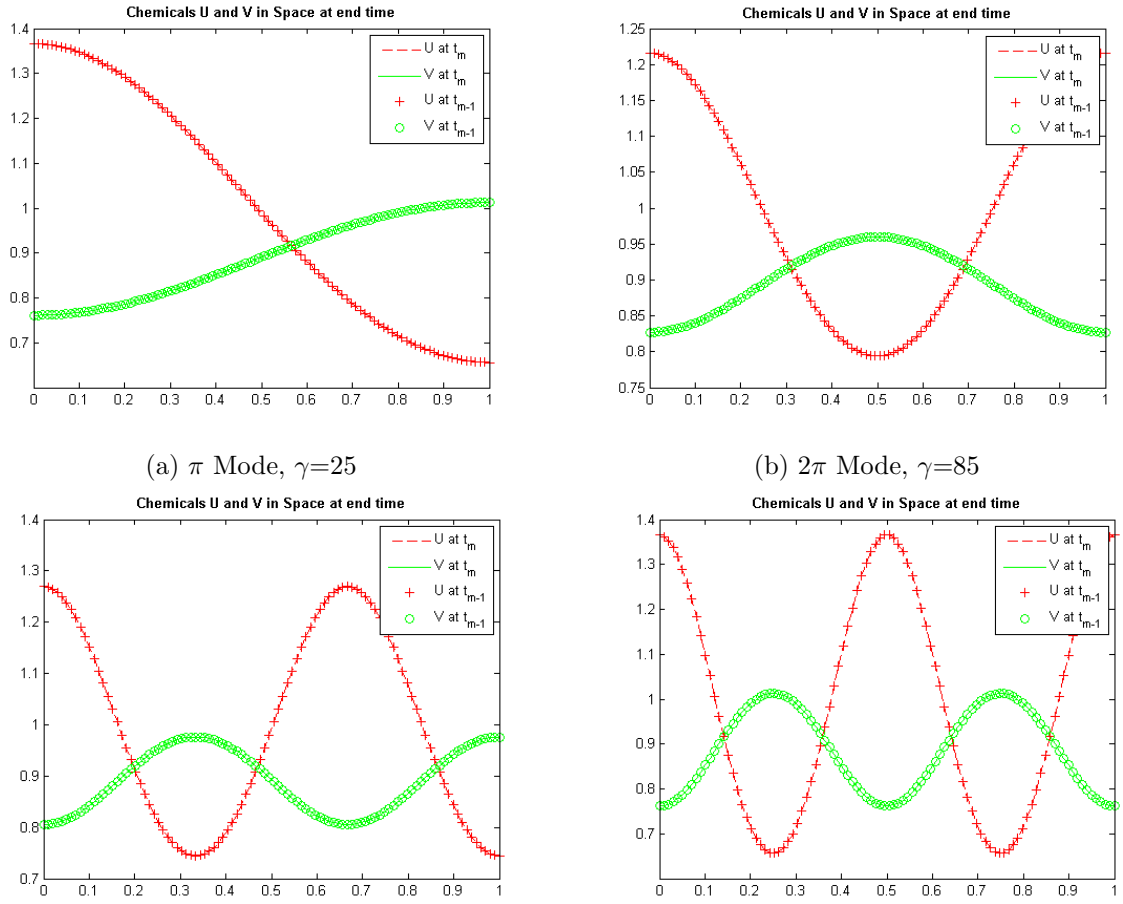
The mode isolation tests of both discretizations illustrate that the algorithm's resultant patterns respond to the parameter space as predicted. We also observe that the Schnakenberg patterns produced are independent of the discretization used.

We next estimate error and convergence for the patterns produced using Schnakenberg kinetics. To estimate the error for simulations we treat the computer run with the finest spatial mesh, corresponding to N_{exact}, as an exact solution. Then we estimate the error of a simulation on a rougher spatial mesh, corresponding to N_{rough}, using two methods. The first measure of error, the maximum error, is calculated by defining an evaluation mesh of the spatial domain as follows

$$h_{eval} = h_{exact}/10,\ N_{eval} = N_{exact} * 10\,,$$
$$x_{i,eval} = \alpha + (i-1)h_{eval},\ i = 1, 2, \ldots, N_{eval} + 1\,.$$

Using this evaluation mesh we find the maximum error at time t_m as

$$Error_{max} = \text{Max}\left\{\left|U^m_{exact}(x_{i,eval}) - U^m_{rough}(x_{i,eval})\right| : i = 1, 2, \ldots, N_{eval} + 1\right\}\,.$$



(a) π Mode, γ=25

(b) 2π Mode, γ=85

(c) 3π Mode, γ=200

(d) 4π Mode, γ=400

Figure 3.3: Crank-Nicolson FEM on a fixed domain and with Schnakenberg kinetics. Mode isolation tests with parameters: $a = 0.1, b = 0.9, d = 10$.

The second measure of error, the L^2 error, is approximated using the evaluation mesh as well. We denote a trapezoidal quadrature to approximate an integral as $Quad(f(x), \alpha, \beta) \approx \int_\alpha^\beta f(x)dx$. Thus we write our approximation of the L^2 error as

$$Error_{L^2} = \sqrt{Quad\left(\left\{U^m_{exact}(x) - U^m_{rough}(x)\right\}^2\right), \alpha, \beta)}\,.$$

In Tables 3.1 and 3.2 we approximate the error for several computer runs using both Backward Euler and Crank-Nicolson discretization. All computer runs were conducted using parameter values of $a = 0.1, b = 0.9, d = 10, \gamma = 35, T = 5$. We also take a Crank-Nicolson run with $N = 1600$ as an exact solution for the error calculations.

Table 3.1: Approximation Error, Backward Euler Discretization

N	$Error_{Max}$	$Error_{L^2}$
40	$2.3968e-04$	$9.7271e-05$
80	$6.9860e-05$	$3.4253e-05$
100	$5.1824e-05$	$2.6094e-05$
160	$2.8644e-05$	$1.5668e-05$
200	$2.1938e-05$	$1.2501e-05$
400	$1.0039e-05$	$6.3294e-06$
800	$4.8410e-06$	$3.2178e-06$
1600	$2.2342e-06$	$1.6331e-06$

Table 3.2: Approximation Error, Crank-Nicolson Discretization

N	$Error_{Max}$	$Error_{L^2}$
40	$3.5680e-04$	$9.8558e-05$
80	$8.9056e-05$	$2.4645e-05$
100	$5.6897e-05$	$1.5763e-05$
160	$2.2063e-05$	$6.1419e-06$
200	$1.4028e-05$	$3.9229e-06$
400	$3.3283e-06$	$9.6729e-07$
800	$6.6195e-07$	$2.2751e-07$

We can also approximate the rates of convergence of the respective discretizations using the estimated errors. Specifically, we approximate the rate of convergence using the formula

$$r \approx \frac{log\left(\frac{error_{2N}}{error_N}\right)}{\log(2)}.$$

Tables 3.4 and 3.5 summarize the rates of convergence for the Backward Euler and Crank-Nicolson runs.

Table 3.3: Convergence, Backward Euler Discretization

N	r_{Max}	r_{L^2}
40	1.7786	1.5057
80	1.2862	1.1283
100	1.2401	1.0615
200	1.1277	0.9820
400	1.0522	0.9759
800	1.1155	0.9784

Table 3.4: Convergence, Crank-Nicolson Discretization

N	r_{Max}	r_{L^2}
40	2.0023	1.9996
80	2.0130	2.0045
100	2.0199	2.0065
200	2.0755	2.0199
400	2.3299	2.0879

We note that Tables 3.4 and 3.5 provide evidence for the motivation of this thesis. Specifically, Crank-Nicolson discretization in conjunction with the novel linearization has yielded second order convergence. Further, we can compare the efficiencies of the two discretizations by calculating a ratio of computer run-times for a given accuracy. For example, if we desire patterns with an accuracy of six decimal digits, then we can choose either the Backward Euler run with $N = 1600$ or the Crank-Nicolson run with $N = 400$. These runs have respective $Error_{L^2}$ of $1.6331e-06$ and $9.6729e-07$ as seen in Tables 3.1 and 3.2. Computer run-times are respectively 2252 seconds and 211 seconds. Thus, the Crank-Nicolson discretization generates a pattern of this accuracy approximately 10.6 times faster.

3.4.3 Gierer-Meinhardt Results

Results of our fixed domain algorithm for Gierer-Meinhardt kinetics shows a pronounced difference in the discretizations. As our algorithm uses approximations to integrals at each time step for these kinetics, it is markedly slower in comparison to the Schnakenberg simulations. For example, with $N = 10$, computation times for Backward Euler and Crank-Nicolson are respectively 178 seconds and 333 seconds. The inherent slowness of this algorithm leads to a desire for efficiency. Figures 3.4 and 3.5 illustrate the patterns modeled for Gierer-Meinhardt kinetics with the two discretizations. For both figures the parameters are fixed as: $a = 0.1$, $b = 1$, $\kappa = 0.5$, $d = 72$, $\gamma = 75$.

Also both graphs correspond to being run to time $t = 7.5$.

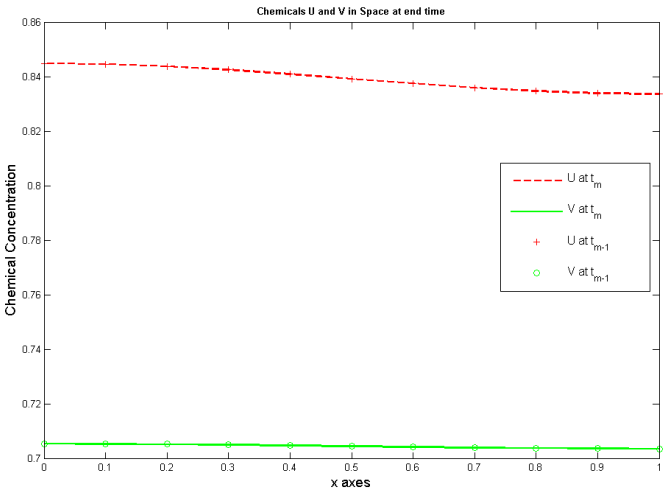


Figure 3.4: Gierer-Meinhardt Pattern Formation, Backward Euler

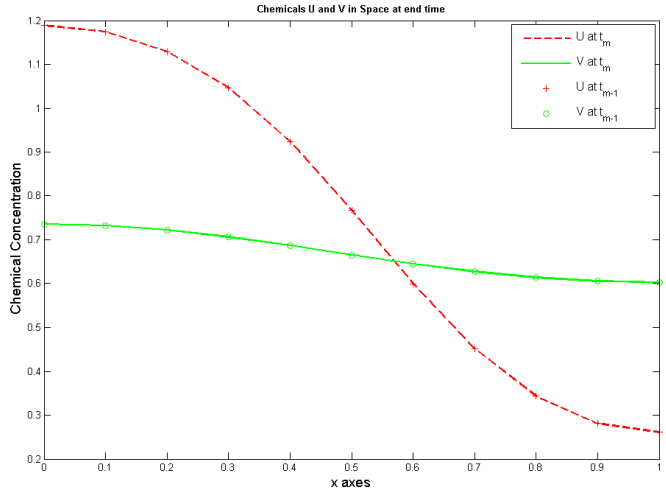


Figure 3.5: Gierer-Meinhardt Pattern Formation, Crank-Nicolson

Comparing these two figures leads to the conclusion that we absolutely want to use Crank-Nicolson discretization for modeling Gierer-Meinhardt kinetics. Several long computational time simulations, i.e. relatively large N, were completed to verify that both discretizations approach the same pattern. Figures 3.6 and 3.7 illustrate these long simulations. For these figures the parameters were again fixed as: $a = 0.1$, $b = 1$, $\kappa = 0.5$, $d = 72$, $\gamma = 75$. For these figures, the end time of the run is $t = 2.5$.

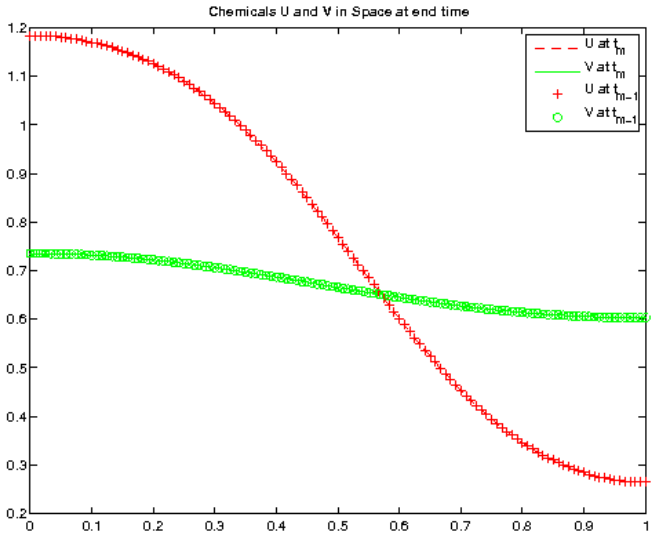


Figure 3.6: Gierer-Meinhardt , Backward Euler, $N = 120$

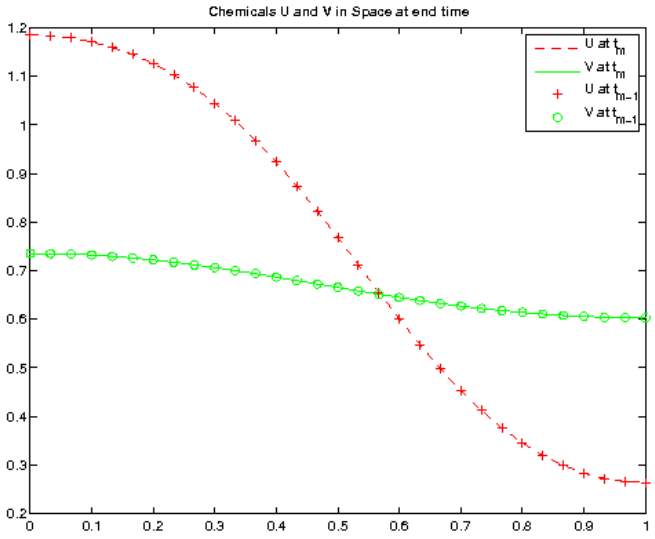


Figure 3.7: Gierer-Meinhardt, Crank-Nicolson, $N = 30$

Figures 3.6 and 3.7 illustrate that the discretizations both approach the same pattern. This lends credence to validation of the algorithm as well.

In the next chapter of this thesis we investigate Turing pattern formation on time dependent spatial domains.

CHAPTER 4

PATTERN FORMATION ON AN EVOLVING DOMAIN

In this chapter we develop an algorithm to model pattern formation on time dependent spatial domains. This algorithm uses a moving finite element method [5, 11]. Similar to our work on the fixed domain algorithm, we use two choices of discretization and linearization. The reaction-diffusion system we use as the mathematical model for pattern generation is given by:

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} + \gamma f_1(u(x,t), v(x,t)),\ x \in [A(t), B(t)]\ , t \in [0,T]\,, \tag{4.1}$$

$$\frac{\partial v(x,t)}{\partial t} = d\frac{\partial^2 v(x,t)}{\partial x^2} + \gamma f_2(u(x,t), v(x,t)),\ x \in [A(t), B(t)]\,, t \in [0,T]\,, \tag{4.2}$$

$$\frac{\partial u(A(t),t)}{\partial x} = \frac{\partial u(B(t),t)}{\partial x} = \frac{\partial v(A(t),t)}{\partial x} = \frac{\partial v(B(t),t)}{\partial x} = 0,\ t \in (0,T)\,, \tag{4.3}$$

$$u(x,0) = g_1(x), \quad v(x,0) = g_2(x),\ x \in [A(0), B(0)]\,, \tag{4.4}$$

where $f_1(u,v), f_2(u,v)$ are given reaction kinetics of the types from Chapter 2, and $g_1(x), g_2(x)$ are given initial conditions.

4.1 Variational Formulation

A finite element method to numerically simulate equations (4.1)-(4.3) begins with a variational formulation. For our continuous model, we seek each component solution in the Sobolev space $\mathcal{V}(t) = H^1(A(t), B(t))$, comprising all weakly differentiable functions on $(A(t), B(t))$. Then, to find the variational formulation of equations (4.1) and (4.2) we now multiply each by a test function $w \in \mathcal{V}(t)$ and integrate over the spatial domain $x \in (A(t), B(t))$.

$$\int_{A(t)}^{B(t)} \frac{\partial u}{\partial t} w - \int_{A(t)}^{B(t)} \frac{\partial^2 u}{\partial x^2} w - \int_{A(t)}^{B(t)} \gamma f_1(u,v) w = 0\,,\ \forall w \in \mathcal{V}(t)\,, \tag{4.5}$$

$$\int_{A(t)}^{B(t)} \frac{\partial v}{\partial t} w - \int_{A(t)}^{B(t)} d\frac{\partial^2 v}{\partial x^2} w - \int_{A(t)}^{B(t)} \gamma f_2(u,v) w = 0\,,\ \forall w \in \mathcal{V}(t)\,. \tag{4.6}$$

We now consider the boundary conditions, equation (4.3). Using equation (4.3) while integrating by parts for equations (4.5) and (4.6) yields

$$\int_{A(t)}^{B(t)} \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) w = \frac{\partial u}{\partial x} w\Big|_{A(t)}^{B(t)} - \int_{A(t)}^{B(t)} \frac{\partial u}{\partial x}\frac{\partial w}{\partial x}\,,$$
$$= \frac{\partial u(B(t),t)}{\partial x} w(B(t)) - \frac{\partial u(A(t),t)}{\partial x} w(A(t)) - \int_{A(t)}^{B(t)} \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = -\int_{A(t)}^{B(t)} \frac{\partial u}{\partial x}\frac{\partial w}{\partial x}\,,$$
$$\int_{A(t)}^{B(t)} d\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x}\right) w = d\,\frac{\partial v}{\partial x} w\Big|_{A(t)}^{B(t)} - d\int_{A(t)}^{B(t)} \frac{\partial v}{\partial x}\frac{\partial w}{\partial x}\,,$$
$$= d\frac{\partial v(B(t),t)}{\partial x} w(B(t)) - d\frac{\partial v(A(t),t)}{\partial x} w(A(t)) - d\int_{A(t)}^{B(t)} \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = -d\int_{A(t)}^{B(t)} \frac{\partial v}{\partial x}\frac{\partial w}{\partial x}\,.$$

With these simplifications applied to equations (4.5) and (4.6) we obtain

$$\int_{A(t)}^{B(t)} \frac{\partial u}{\partial t} w + \int_{A(t)}^{B(t)} \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = \int_{A(t)}^{B(t)} \gamma f_1(u,v) w, \quad \forall w \in \mathcal{V}(t)\,, \tag{4.7}$$

$$\int_{A(t)}^{B(t)} \frac{\partial v}{\partial t} w + d\int_{A(t)}^{B(t)} \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = \int_{A(t)}^{B(t)} \gamma f_2(u,v) w, \quad \forall w \in \mathcal{V}(t)\,. \tag{4.8}$$

Equations (4.7) and (4.8) are the variational formulations for (4.1) and (4.2) respectively.

4.2 Moving Finite Element Method

In this section we discuss the background and theory for a moving finite element method. As with the standard finite element method, we begin by establishing meshes. We establish a uniform mesh of the temporal interval:

$$t_1 = 0, \quad t_{M+1} = T, \quad \triangle t = \frac{T}{M}\,,$$
$$t_m = (m-1)\triangle T: \quad m \in \{1, 2, 3, \ldots, M+1\}\,.$$

Also, for each t, $t \in \{t_1, t_2, \ldots, t_{M+1}\}$ we establish a uniform mesh of the time dependent spatial domain $[A(t), B(t)]$:

$$a_1(t) = A(t), \quad a_{N+1}(t) = B(t), \quad h(t) = \frac{a_{N+1}(t) - a_1(t)}{N}\,,$$
$$a_n(t) = a_1(t) + (n-1)h(t): \quad n \in \{1, 2, \ldots, N+1\}\,.$$

We further define a vector $\mathbf{a}(t)$ of spatial node positions, such that

$$\mathbf{a}(t) = [a_1(t) \quad a_2(t) \quad \cdots \quad a_{N+1}(t)]^T\,.$$

As in the case of a fixed spatial domain FEM, we define intervals of the spatial domain in order to define basis functions with compact support. In this case the intervals depend on time

$$I_j(t) = [a_j(t), a_{j+1}(t)]\,. \tag{4.9}$$

We also define the subspace $\mathcal{V}_h(t) \subset \mathcal{V}(t)$:

$$\mathcal{V}_h(t) = \text{Span}\{\alpha_i(x, \mathbf{a}(t)),\, i = 1, 2, \ldots, N+1\}\,,$$

where we define the basis functions $\alpha_i(x, \mathbf{a}(t))$ as

$$\alpha_1(x, \mathbf{a}(t)) = \begin{cases} \frac{a_2(t)-x}{a_2(t)-a_1(t)} & , \quad x \in I_1(t) \\ 0 & , \quad \text{otherwise} \end{cases}\,,$$

$$\alpha_j(x, \mathbf{a}(t)) = \begin{cases} \frac{x-a_{j-1}(t)}{a_j(t)-a_{j-1}(t)} & , \quad x \in I_{j-1}(t) \\ \frac{a_{j+1}(t)-x}{a_{j+1}(t)-a_j(t)} & , \quad x \in I_j(t) \\ 0 & , \quad \text{otherwise} \end{cases} \quad , \quad j \in \{2, 3, \ldots, N\}\,,$$

$$\alpha_{N+1}(x, \mathbf{a}(t)) = \begin{cases} \frac{x-a_N(t)}{a_{N+1}(t)-a_N(t)} & , \quad x \in I_N(t) \\ 0 & , \quad \text{otherwise} \end{cases}\,.$$

We now write FEM approximations of $u(x,t), v(x,t)$ in the finite dimensional space $\mathcal{V}_h(t)$ as

$$U(x,t) = \sum_{i=1}^{N+1} k_i(t)\alpha_i(x, \mathbf{a}(t))\,, \tag{4.10}$$

$$V(x,t) = \sum_{i=1}^{N+1} l_i(t)\alpha_i(x, \mathbf{a}(t))\,. \tag{4.11}$$

where the coefficients $k_i(t), l_i(t)$ are to be found. Investigation of the approximation (4.10), and specifically the temporal derivative of $U(x,t)$ shows:

$$\begin{aligned} \frac{\partial U(x,t)}{\partial t} &= \frac{\partial}{\partial t}\left(\sum_{i=1}^{N+1} k_i(t)\alpha_i(x, \mathbf{a}(t))\right)\,, \\ &= \sum_{i=1}^{N+1} \frac{\partial}{\partial t}\left[k_i(t)\alpha_i(x, \mathbf{a}(t))\right]\,, \\ &= \sum_{i=1}^{N+1} \left(\dot{k}_i(t)\alpha_i(x, \mathbf{a}(t)) + k_i(t)\frac{\partial}{\partial t}\alpha_i(x, \mathbf{a}(t))\right)\,, \\ &= \sum_{i=1}^{N+1} \dot{k}_i(t)\alpha_i(x, \mathbf{a}(t)) + \sum_{i=1}^{N+1} k_i(t)\frac{\partial \alpha_i(x, \mathbf{a}(t))}{\partial \mathbf{a}(t)}\frac{\partial \mathbf{a}(t)}{\partial t}\,, \end{aligned} \tag{4.12}$$

where the overdot is used to denote a temporal derivative. We note that on the last line of equation (4.12) the first term on the right hand side (RHS) is the derivative we would encounter in a fixed spatial domain FEM. The second term on the RHS is an additional derivative we encounter due to the time dependent spatial domain. We can expand this additional term as

$$\sum_{i=1}^{N+1} k_i(t) \frac{\partial \alpha_i(x, \mathbf{a}(t))}{\partial \mathbf{a}(t)} \frac{\partial \mathbf{a}(t)}{\partial t} = \sum_{i=1}^{N+1} k_i(t) \sum_{j=1}^{N+1} \frac{\partial \alpha_i(x, \mathbf{a}(t))}{\partial a_j(t)} \frac{\partial a_j(t)}{\partial t} \,. \tag{4.13}$$

If we denote

$$\nabla_{\mathbf{a}} \alpha_i = \begin{bmatrix} \frac{\partial \alpha_i}{\partial a_1} & \frac{\partial \alpha_i}{\partial a_2} & \cdots & \frac{\partial \alpha_i}{\partial a_{N+1}} \end{bmatrix}^T ,$$
$$\dot{\mathbf{a}} = \begin{bmatrix} \frac{\partial a_1}{\partial t} & \frac{\partial a_2}{\partial t} & \cdots & \frac{\partial a_{N+1}}{\partial t} \end{bmatrix}^T ,$$

We can then write equation (4.13) as

$$\begin{aligned} &\sum_{i=1}^{N+1} k_i(t) \sum_{j=1}^{N+1} \frac{\partial \alpha_i(x, \mathbf{a}(t))}{\partial a_j(t)} \frac{\partial a_j(t)}{\partial t} = \sum_{i=1}^{N+1} k_i \sum_{j=1}^{N+1} [\nabla_{\mathbf{a}} \alpha_i]_j [\dot{\mathbf{a}}]_j \,, \\ &= \sum_{i=1}^{N+1} \sum_{j=1}^{N+1} k_i [\nabla_{\mathbf{a}} \alpha_i]_j [\dot{\mathbf{a}}]_j = \sum_{j=1}^{N+1} \sum_{i=1}^{N+1} k_i [\nabla_{\mathbf{a}} \alpha_i]_j [\dot{\mathbf{a}}]_j \,, \\ &= \sum_{j=1}^{N+1} [\dot{\mathbf{a}}]_j \sum_{i=1}^{N+1} k_i [\nabla_{\mathbf{a}} \alpha_i]_j = \sum_{j=1}^{N+1} [\dot{\mathbf{a}}]_j \beta_j = \sum_{i=1}^{N+1} [\dot{\mathbf{a}}]_i \beta_i \,. \end{aligned} \tag{4.14}$$

We can further expand β_i from equation (4.14) as

$$\begin{aligned} \beta_i &= \sum_{j=1}^{N+1} k_j [\nabla_{\mathbf{a}} \alpha_j]_i = \sum_{j=1}^{N+1} [\nabla_{\mathbf{a}} (k_j \alpha_j)]_i = \left[\nabla_{\mathbf{a}} \sum_{j=1}^{N+1} k_j \alpha_j \right]_i , \\ &= [\nabla_{\mathbf{a}} U(x,t)]_i = \frac{\partial U(x,t)}{\partial a_i} \,. \end{aligned}$$

As noted in [3], in multiple spatial dimensions we have that

$$\beta_i = \frac{\partial U}{\partial a_i} = -\alpha_i \nabla_{\mathbf{x}} U \,. \tag{4.15}$$

Thus in one spatial dimension we have:

$$\beta_i = -\alpha_i(x, \mathbf{a}(t)) \frac{\partial U(x,t)}{\partial x}, \quad [\dot{\mathbf{a}}]_i = \frac{\partial a_i(t)}{\partial t} = \dot{a}_i(t) \,. \tag{4.16}$$

As an aside, while $[\dot{\mathbf{a}}]_i$ and β_i are scalars in a one spatial dimension problem, these terms are more

complex in multiple spatial dimensions. For example, in two spatial dimensions these terms take the vector forms [11] of

$$\dot{\mathbf{a}}_i = [\dot{x}_i \, \dot{y}_i]^T \,, \quad \frac{\partial U(\mathbf{x},t)}{\partial \mathbf{x}} = [U_x \, U_y]^T \,.$$

Using equation (4.16), we write (4.12) as

$$\begin{aligned}
\frac{\partial U(x,t)}{\partial t} &= \sum_{i=1}^{N+1} \dot{k}_i(t)\alpha_i(x,\mathbf{a}(t)) + \sum_{i=1}^{N+1} [\dot{\mathbf{a}}]_i \, \beta_i \,, \\
&= \sum_{i=1}^{N+1} \dot{k}_i(t)\alpha_i(x,\mathbf{a}(t)) - \sum_{i=1}^{N+1} \dot{a}_i(t)\alpha_i(x,\mathbf{a}(t))\frac{\partial U(x,t)}{\partial x} \,, \\
&= \sum_{i=1}^{N+1} \left(\dot{k}_i(t) - \dot{a}_i(t)\frac{\partial U(x,t)}{\partial x} \right) \alpha_i(x,\mathbf{a}(t)) \,. \qquad (4.17)
\end{aligned}$$

Equation (4.17) allows us to discretize the temporal derivatives of our variational formulation on the time dependent spatial domain.

4.3 Moving Finite Element Method: Schnakenberg Kinetics

In this section we describe the discretizations, both Backward Euler and Crank-Nicolson, and the respective linearizations that enable us to write the variational formulation as linear systems. Specifically, we deal with the variational formulation with Schnakenberg kinetics. The variational formulation of interest is thus given by

$$\int_{A(t)}^{B(t)} \frac{\partial u}{\partial t} w + \int_{A(t)}^{B(t)} \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} = \int_{A(t)}^{B(t)} \gamma(a - u + u^2 v) w, \quad \forall w \in \mathcal{V}(t) \,, \qquad (4.18)$$

$$\int_{A(t)}^{B(t)} \frac{\partial v}{\partial t} w + d\int_{A(t)}^{B(t)} \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} = \int_{A(t)}^{B(t)} \gamma(b - u^2 v) w, \quad \forall w \in \mathcal{V}(t) \,. \qquad (4.19)$$

We next approximate u, v in $\mathcal{V}_h(t)$, as seen in equation (4.10) and (4.11) and also use

$$\langle f, g \rangle_t = \int_{A(t)}^{B(t)} f(x)g(x) \, \mathrm{d}x, \quad \mathcal{A}_t(f,g) = \int_{A(t)}^{B(t)} \frac{\partial f(x)}{\partial x}\frac{\partial g(x)}{\partial x} \, \mathrm{d}x \,.$$

We thus write equations (4.18) and (4.19) as

$$\begin{aligned}
&\left\langle \frac{\partial U}{\partial t}, w \right\rangle_t + \mathcal{A}_t(U,w) = \left\langle \gamma(a - U + U^2 V), w \right\rangle_t \,, \qquad (4.20) \\
&\left\langle \frac{\partial V}{\partial t}, w \right\rangle_t + d\mathcal{A}_t(V,w) = \left\langle \gamma(b - U^2 V), w \right\rangle_t \,, \qquad (4.21) \\
&x \in [A(t), B(t)] \,, t \in [0,T] \,, w \in \mathcal{V}_h(t) \,.
\end{aligned}$$

Replacing the temporal derivatives with their expansions, via equation (4.17), yields

$$\left\langle \sum_{i=1}^{N+1} \left(\dot{k}_i(t) - \dot{a}_i(t) \frac{\partial U(x,t)}{\partial x} \right) \alpha_i(x, \mathbf{a}(t)), w \right\rangle_t + \mathcal{A}_t \left(U(x,t), w \right) = \left\langle \gamma(a - U + U^2 V), w \right\rangle_t , \quad (4.22)$$

$$\left\langle \sum_{i=1}^{N+1} \left(\dot{l}_i(t) - \dot{a}_i(t) \frac{\partial V(x,t)}{\partial x} \right) \alpha_i(x, \mathbf{a}(t)), w \right\rangle_t + d\mathcal{A}_t \left(V(x,t), w \right) = \left\langle \gamma(b - U^2 V), w \right\rangle_t , \quad (4.23)$$

$x \in [A(t), B(t)]$, $t \in [0, T]$, $w \in \mathcal{V}_h(t)$.

To obtain a fully discrete system for computing solutions let us denote for a fixed time of the temporal mesh $t_m \in [0, T]$:

$$\begin{aligned} & w^m = w \in \mathcal{V}_h(t_m),\ \alpha_i(x, \mathbf{a}(t_m)) = \alpha_i^m(x),\ [\mathbf{a}(t_m)]_i = a_i^m , \\ & U(x, t_m) = \sum_{i=1}^{N+1} k_i(t_m) \alpha_i(x, \mathbf{a}(t_m)) = \sum_{i=1}^{N+1} k_i^m \alpha_i^m(x) = U^m(x) , \\ & V(x, t_m) = \sum_{i=1}^{N+1} l_i(t_m) \alpha_i(x, \mathbf{a}(t_m)) = \sum_{i=1}^{N+1} l_i^m \alpha_i^m(x) = V^m(x) . \end{aligned}$$

Using the above notation we can conclude that for t_1, $U^1(x), V^1(x)$ are given by the initial conditions, equation (4.4), approximated in the $\mathcal{V}_h$ space:

$$\begin{aligned} & U^1(x) = \sum_{i=1}^{N+1} k_i(t_1) \alpha_i(x, \mathbf{a}(t_1)),\ k_i(t_1) = g_1(a_i(t_1)) , \\ & V^1(x) = \sum_{i=1}^{N+1} l_i(t_1) \alpha_i(x, \mathbf{a}(t_1)),\ k_i(t_1) = g_2(a_i(t_1)) . \end{aligned}$$

4.3.1 Backward Euler Finite Element Method

A Backward Euler finite element method for equations (4.22) and (4.23) is given by

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(k_i^m \alpha_i^m(x) - k_i^{m-1} \alpha_i^m(x) \right) - \left(a_i^m \frac{\partial U^m(x)}{\partial x} \alpha_i^m(x) - a_i^{m-1} \frac{\partial U^m(x)}{\partial x} \alpha_i^m(x) \right)}{\triangle t} \right\}, w^m \right\rangle_t$$

$$+ \mathcal{A}_t \left(U^m(x), w^m \right) = \left\langle \gamma \left(a - U^m(x) + \left(U^m(x) \right)^2 V^m(x) \right), w^m \right\rangle_t , \quad (4.24)$$

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(l_i^m \alpha_i^m(x) - l_i^{m-1} \alpha_i^m(x) \right) - \left(a_i^m \frac{\partial V^m(x)}{\partial x} \alpha_i^m(x) - a_i^{m-1} \frac{\partial V^m(x)}{\partial x} \alpha_i^m(x) \right)}{\triangle t} \right\}, w^m \right\rangle_t$$

$$+ d\mathcal{A}_t \left(V^m(x), w \right) = \left\langle \gamma \left(b - \left(U^m(x) \right)^2 V^m(x) \right), w^m \right\rangle_t , \quad (4.25)$$

$x \in [A(t_m), B(t_m)]$, $m \in \{2, 3, \ldots, M+1\}$, $w^m \in \mathcal{V}_h(t_m)$.

We next linearize the $(U^m)^2$ terms of equations (4.24) and (4.25). Namely, we approximate

$$(U^m)^2 V^m = \left(\sum_{i=1}^{N+1} k_i^m \alpha_i^m\right)^2 \left(\sum_{i=1}^{N+1} l_i^m \alpha_i^m\right) \approx \left(\sum_{i=1}^{N+1} k_i^{m-1} \alpha_i^m\right)^2 \left(\sum_{i=1}^{N+1} l_i^m \alpha_i^m\right).$$

Using this linearization, we can write equations (4.24) and (4.25) as

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(k_i^m \alpha_i^m(x) - k_i^{m-1} \alpha_i^m(x)\right) - \left(a_i^m \frac{\partial U^m(x)}{\partial x} \alpha_i^m(x) - a_i^{m-1} \frac{\partial U^m(x)}{\partial x} \alpha_i^m(x)\right)}{\triangle t} \right\}, w^m \right\rangle_t$$
$$+ \mathcal{A}_t \left(U^m(x), w^m\right) = \left\langle \gamma \left(a - U^m(x) + \left(\sum_{i=1}^{N+1} k_i^{m-1} \alpha_i^m\right)^2 \left(\sum_{i=1}^{N+1} l_i^m \alpha_i^m\right) \right), w^m \right\rangle_t, \tag{4.26}$$

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(l_i^m \alpha_i^m(x) - l_i^{m-1} \alpha_i^m(x)\right) - \left(a_i^m \frac{\partial V^m(x)}{\partial x} \alpha_i^m(x) - a_i^{m-1} \frac{\partial V^m(x)}{\partial x} \alpha_i^m(x)\right)}{\triangle t} \right\}, w^m \right\rangle_t$$
$$+ d\mathcal{A}_t \left(V^m(x), w\right) = \left\langle \gamma \left(b - \left(\sum_{i=1}^{N+1} k_i^{m-1} \alpha_i^m\right)^2 \left(\sum_{i=1}^{N+1} l_i^m \alpha_i^m\right) \right), w^m \right\rangle_t, \tag{4.27}$$

$$x \in [A(t_m), B(t_m)], m \in \{2, 3, \ldots, M+1\}, w^m \in \mathcal{V}_h(t_m).$$

Simplification is now conducted using the bilinearity of the operations $\langle \cdot, \cdot \rangle_t$, $\mathcal{A}_t$. Also, as we have $w^m \in \mathcal{V}_h(t_m)$ we can restrict it to α_j^m, $j \in \{1, 2, \ldots, N+1\}$. Thus we write equations (4.26) and (4.27) as

$$(1 + \gamma \triangle t) \sum_{i=1}^{N+1} k_i^m \left\langle \alpha_i^m, \alpha_j^m \right\rangle_t - \sum_{i=1}^{N+1} k_i^m \left\langle \frac{\partial \alpha_i^m}{\partial x} \sum_{r=1}^{N+1} \left(a_r^m - a_r^{m-1}\right) \alpha_r^m, \alpha_j^m \right\rangle_t$$
$$+ \triangle t \sum_{i=1}^{N+1} k_i^m \mathcal{A}_t \left(\alpha_i^m, \alpha_j^m\right) = \gamma \triangle t \left\langle a, \alpha_j^m \right\rangle_t + \sum_{i=1}^{N+1} k_i^{m-1} \left\langle \alpha_i^m, \alpha_j^m \right\rangle_t$$
$$+ \gamma \triangle t \sum_{i=1}^{N+1} l_i^m \left\langle \left(\sum_{r=1}^{N+1} k_r^{m-1} \alpha_r^m\right)^2 \alpha_i^m, \alpha_j^m \right\rangle_t, \tag{4.28}$$

$$\sum_{i=1}^{N+1} l_i^m \left\langle \alpha_i^m, \alpha_j^m \right\rangle_t - \sum_{i=1}^{N+1} l_i^m \left\langle \frac{\partial \alpha_i^m}{\partial x} \sum_{r=1}^{N+1} \left(a_r^m - a_r^{m-1}\right) \alpha_r^m, \alpha_j^m \right\rangle_t$$
$$+ d \triangle t \sum_{i=1}^{N+1} l_i^m \mathcal{A}_t \left(\alpha_i^m, \alpha_j^m\right) + \gamma \triangle t \sum_{i=1}^{N+1} l_i^m \left\langle \left(\sum_{r=1}^{N+1} k_r^{m-1} \alpha_r^m\right)^2 \alpha_i^m, \alpha_j^m \right\rangle_t$$
$$= \gamma \triangle t \left\langle b, \alpha_j^m \right\rangle_t + \sum_{i=1}^{N+1} l_i^{m-1} \left\langle \alpha_i^m, \alpha_j^m \right\rangle_t, \tag{4.29}$$

$$x \in [A(t_m), B(t_m)], m \in \{2, 3, \ldots, M+1\}, j \in \{1, 2, \ldots, N+1\}.$$

Next we define the following vectors and matrices:

$$
\begin{aligned}
&[\mathbf{A^m}]_{i,j} = \mathcal{A}_t\left(\alpha_i^m(x), \alpha_j^m(x)\right), [\mathbf{M_1^m}]_{i,j} = \left\langle \alpha_i^m(x), \alpha_j^m(x) \right\rangle_t, \\
&[\mathbf{M_2^m}]_{i,j} = \left\langle \frac{\partial \alpha_i^m(x)}{\partial x} \sum_{r=1}^{N+1} \left(a_r^m - a_r^{m-1}\right) \alpha_r^m(x), \alpha_j^m(x) \right\rangle_t, \\
&[\mathbf{Q^m}]_{i,j} = \left\langle \left(\sum_{r=1}^{N+1} k_r^{m-1} \alpha_r^m \right)^2 \alpha_i^m, \alpha_j^m \right\rangle_t, \\
&\mathbf{k^m} = \left[k_1^m\, k_2^m\, \cdots\, k_{N+1}^m\right]^T, \mathbf{l^m} = \left[l_1^m\, l_2^m\, \cdots\, l_{N+1}^m\right]^T, \\
&\mathbf{z_1^m} = \left[< a, \alpha_1^m >_t < a, \alpha_2^m >_t \cdots < a, \alpha_{N+1}^m >_t\right]^T, \\
&\mathbf{z_2^m} = \left[< b, \alpha_1^m >_t < b, \alpha_2^m >_t \cdots < b, \alpha_{N+1}^m >_t\right]^T.
\end{aligned}
$$

Using these matrices and vectors we write equations (4.28) and (4.29) as

$$
\begin{aligned}
&\left\{(1+\gamma\triangle t)\mathbf{M_1^m} - \mathbf{M_2^m} + \triangle t \mathbf{A^m}\right\} \mathbf{k^m} = \gamma \triangle t \mathbf{z_1} + \mathbf{M_1^m k^{m-1}} + \gamma \triangle t \mathbf{Q^m l^m}, \qquad (4.30) \\
&\left\{\mathbf{M_1^m} - \mathbf{M_2^m} + d\triangle t \mathbf{A} + \gamma \triangle t \mathbf{Q^m}\right\} \mathbf{l^m} = \gamma \triangle t \mathbf{z_2} + \mathbf{M_1^m l^{m-1}}, \qquad (4.31) \\
&m \in \{2, 3, \ldots, N+1\}.
\end{aligned}
$$

Equations (4.30) and (4.31) constitute a linear system for the FEM approximations of equations (4.18) and (4.19). An algorithm that implements equations (4.30) and (4.31) has been written, and its results are discussed later in this chapter.

4.3.2 Crank-Nicolson Finite Element Method

A Crank-Nicolson finite element method for equations (4.22) and (4.23) for a given time t_m can be written as

$$
\begin{aligned}
&\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(k_i^m - k_i^{m-1}\right)}{\triangle t} \alpha_i^{m-1/2} - \frac{\left(a_i^m - a_i^{m-1}\right)}{\triangle t} \frac{\partial U^{m-1/2}}{\partial x} \alpha_i^{m-1/2} \right\}, w^{m-1/2} \right\rangle_t \\
&+ \mathcal{A}_t\left(U^{m-1/2}, w^{m-1/2}\right) = \left\langle \gamma \left(a - U^{m-1/2} + \left(U^{m-1/2}\right)^2 V^{m-1/2} \right), w^{m-1/2} \right\rangle_t, \qquad (4.32) \\
&\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(l_i^m - l_i^{m-1}\right)}{\triangle t} \alpha_i^{m-1/2} - \frac{\left(a_i^m - a_i^{m-1}\right)}{\triangle t} \frac{\partial V^{m-1/2}}{\partial x} \alpha_i^{m-1/2} \right\}, w^{m-1/2} \right\rangle_t \\
&+ d\mathcal{A}_t\left(V^{m-1/2}, w^{m-1/2}\right) = \left\langle \gamma \left(b - \left(U^{m-1/2}\right)^2 V^{m-1/2} \right), w^{m-1/2} \right\rangle_t, \qquad (4.33) \\
&x \in \left[A(t_{m-1/2}), B(t_{m-1/2})\right], m \in \{2, 3, \ldots, M+1\}, w^{m-1/2} \in \mathcal{V}_h(t_{m-1/2}).
\end{aligned}
$$

We approximate the linear terms of $U^{m-1/2}$, $V^{m-1/2}$ as

$$U^{m-1/2} \approx \sum_{i=1}^{N+1} \left(\frac{k_i^m + k_i^{m-1}}{2} \right) \alpha_i(x, t_{m-1/2}),\ V^{m-1/2} \approx \sum_{i=1}^{N+1} \left(\frac{l_i^m + l_i^{m-1}}{2} \right) \alpha_i(x, t_{m-1/2}) \,. \quad (4.34)$$

Using equation (4.34) to expand linear terms of $U^{m-1/2}, V^{m-1/2}$ and restricting $w^{m-1/2} \in \mathcal{V}_h(t_{m-1/2})$ to $\alpha_j^{m-1/2}$, $j \in \{1, 2, \ldots, N+1\}$ yields

$$\begin{aligned}
&\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(k_i^m - k_i^{m-1}\right)}{\triangle t} {\alpha_i}^{m-1/2} - \frac{\left(a_i^m - a_i^{m-1}\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{k_r^m + k_r^{m-1}}{2} \frac{\partial \alpha_r^{m-1/2}}{\partial x} \right) \right. \right. \\
&\left. \left. *\alpha_i^{m-1/2} \right\}, \alpha_j^{m-1/2} \right\rangle_t + \mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{k_i^m + k_i^{m-1}}{2} \alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right) \\
&= \left\langle \gamma \left(a - \sum_{i=1}^{N+1} \frac{k_i^m + k_i^{m-1}}{2} \alpha_i^{m-1/2} + \left(U^{m-1/2}\right)^2 \sum_{i=1}^{N+1} \frac{l_i^m + l_i^{m-1}}{2} \alpha_i^{m-1/2} \right), \alpha_j^{m-1/2} \right\rangle_t , \quad (4.35) \\
&\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(l_i^m - l_i^{m-1}\right)}{\triangle t} {\alpha_i}^{m-1/2} - \frac{\left(a_i^m - a_i^{m-1}\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{l_r^m + l_r^{m-1}}{2} \frac{\partial \alpha_r^{m-1/2}}{\partial x} \right) \right. \right. \\
&\left. \left. *\alpha_i^{m-1/2} \right\}, \alpha_j^{m-1/2} \right\rangle_t + d\mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{l_i^m + l_i^{m-1}}{2} \alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right) \\
&= \left\langle \gamma \left(b - \left(U^{m-1/2}\right)^2 \sum_{i=1}^{N+1} \frac{l_i^m + l_i^{m-1}}{2} \alpha_i^{m-1/2} \right), \alpha_j^{m-1/2} \right\rangle_t , \quad (4.36) \\
&x \in \left[A(t_{m-1/2}), B(t_{m-1/2}) \right] , m \in \{2, 3, \ldots, M+1\} , j \in \{1, 2, \ldots, N+1\} .
\end{aligned}$$

Next, we linearize the $\left(U^{m-1/2}\right)^2$ terms in equations (4.35) and (4.36) as follows:

$$\left(\sum_{i=1}^{N+1} k_i^{m-1/2} \alpha_i^{m-1/2} \right)^2 \approx \left(\sum_{i=1}^{N+1} \frac{3k_i^{m-1} - k_i^{m-2}}{2} \alpha_i^{m-1/2} \right)^2 .$$

As we demonstrated in the fixed spatial domain case, this linearization is $\mathcal{O}(\triangle t)^2$ accurate. This linearization also restricts the system of equations to t_m, $m \in \{3, 4, \ldots, M+1\}$. We derive separate equations for t_2 later in this section. We thus write equations (4.35) and (4.36) as

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(k_i^m - k_i^{m-1}\right)}{\triangle t} \alpha_i^{m-1/2} - \frac{\left(a_i^m - a_i^{m-1}\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{k_r^m + k_r^{m-1}}{2} \frac{\partial \alpha_r^{m-1/2}}{\partial x} \right) \right.\right.$$
$$\left.\left. * \alpha_i^{m-1/2} \right\}, \alpha_j^{m-1/2} \right\rangle_t + \mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{k_i^m + k_i^{m-1}}{2} \alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right)$$
$$= \left\langle \gamma \left(a - \sum_{i=1}^{N+1} \frac{k_i^m + k_i^{m-1}}{2} \alpha_i^{m-1/2} + \left(\sum_{i=1}^{N+1} \frac{3k_i^{m-1} - k_i^{m-2}}{2} \alpha_i^{m-1/2} \right)^2 \right.\right.$$
$$\left.\left. * \sum_{i=1}^{N+1} \frac{l_i^m + l_i^{m-1}}{2} \alpha_i^{m-1/2} \right), \alpha_j^{m-1/2} \right\rangle_t , \tag{4.37}$$
$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(l_i^m - l_i^{m-1}\right)}{\triangle t} \alpha_i^{m-1/2} - \frac{\left(a_i^m - a_i^{m-1}\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{l_r^m + l_r^{m-1}}{2} \frac{\partial \alpha_r^{m-1/2}}{\partial x} \right) \right.\right.$$
$$\left.\left. * \alpha_i^{m-1/2} \right\}, \alpha_j^{m-1/2} \right\rangle_t + d\mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{l_i^m + l_i^{m-1}}{2} \alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right)$$
$$= \left\langle \gamma \left(b - \left(\sum_{i=1}^{N+1} \frac{3k_i^{m-1} - k_i^{m-2}}{2} \alpha_i^{m-1/2} \right)^2 \sum_{i=1}^{N+1} \frac{l_i^m + l_i^{m-1}}{2} \alpha_i^{m-1/2} \right), \alpha_j^{m-1/2} \right\rangle_t , \tag{4.38}$$
$$x \in \left[A(t_{m-1/2}), B(t_{m-1/2}) \right] , m \in \{3, 4, \ldots, M+1\} , j \in \{1, 2, \ldots, N+1\} .$$

Simplification is further conducted using the bilinearity of the operations $\langle \cdot, \cdot \rangle_t$, $\mathcal{A}_t$. Grouping terms of equations (4.37) and (4.38) yields

$$\left(1 + \frac{\gamma \triangle t}{2}\right) \sum_{i=1}^{N+1} k_i^m \left\langle \alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right\rangle_t + \left(\frac{\triangle t}{2}\right) \sum_{i=1}^{N+1} k_i^m \mathcal{A}_t \left(\alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right)$$
$$- \left(\frac{1}{2}\right) \sum_{i=1}^{N+1} k_i^m \left\langle \frac{\partial \alpha_i^{m-1/2}}{\partial x} \left\{ \sum_{r=1}^{N+1} \left(a_r^m - a_r^{m-1}\right) \alpha_r^{m-1/2} \right\}, \alpha_j^{m-1/2} \right\rangle_t$$
$$= \left(1 - \frac{\gamma \triangle t}{2}\right) \sum_{i=1}^{N+1} k_i^{m-1} \left\langle \alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right\rangle_t - \left(\frac{\triangle t}{2}\right) \sum_{i=1}^{N+1} k_i^{m-1} \mathcal{A}_t \left(\alpha_i^{m-1/2}, \alpha_j^{m-1/2} \right)$$
$$+ \left(\frac{1}{2}\right) \sum_{i=1}^{N+1} k_i^{m-1} \left\langle \frac{\partial \alpha_i^{m-1/2}}{\partial x} \left\{ \sum_{r=1}^{N+1} \left(a_r^m - a_r^{m-1}\right) \alpha_r^{m-1/2} \right\}, \alpha_j^{m-1/2} \right\rangle_t$$
$$+ \left(\frac{\gamma \triangle t}{8}\right) \sum_{i=1}^{N+1} l_i^m \left\langle \alpha_i^{m-1/2} \left\{ \sum_{r=1}^{N+1} \left(3k_r^{m-1} - k_r^{m-2}\right) \alpha_r^{m-1/2} \right\}^2, \alpha_j^{m-1/2} \right\rangle_t$$

$$+\left(\frac{\gamma\triangle t}{8}\right)\sum_{i=1}^{N+1} l_i^{m-1}\left\langle \alpha_i^{m-1/2}\left\{\sum_{r=1}^{N+1}\left(3k_r^{m-1}-k_r^{m-2}\right)\alpha_r^{m-1/2}\right\}^2,\alpha_j^{m-1/2}\right\rangle_t+(\gamma\triangle t)\left\langle a,\alpha_j^{m-1/2}\right\rangle_t, \tag{4.39}$$

$$\begin{aligned}
&\sum_{i=1}^{N+1} l_i^m\left\langle \alpha_i^{m-1/2},\alpha_j^{m-1/2}\right\rangle_t+\left(\frac{d\triangle t}{2}\right)\sum_{i=1}^{N+1} l_i^m\mathcal{A}_t\left(\alpha_i^{m-1/2},\alpha_j^{m-1/2}\right)\\
&-\left(\frac{1}{2}\right)\sum_{i=1}^{N+1} l_i^m\left\langle \frac{\partial\alpha_i^{m-1/2}}{\partial x}\left\{\sum_{r=1}^{N+1}\left(a_r^m-a_r^{m-1}\right)\alpha_r^{m-1/2}\right\},\alpha_j^{m-1/2}\right\rangle_t\\
&+\left(\frac{\gamma\triangle t}{8}\right)\sum_{i=1}^{N+1} l_i^m\left\langle \alpha_i^{m-1/2}\left\{\sum_{r=1}^{N+1}\left(3k_r^{m-1}-k_r^{m-2}\right)\alpha_r^{m-1/2}\right\}^2,\alpha_j^{m-1/2}\right\rangle_t\\
&=\sum_{i=1}^{N+1} l_i^{m-1}\left\langle \alpha_i^{m-1/2},\alpha_j^{m-1/2}\right\rangle_t-\left(\frac{d\triangle t}{2}\right)\sum_{i=1}^{N+1} l_i^{m-1}\mathcal{A}_t\left(\alpha_i^{m-1/2},\alpha_j^{m-1/2}\right)\\
&+\left(\frac{1}{2}\right)\sum_{i=1}^{N+1} l_i^{m-1}\left\langle \frac{\partial\alpha_i^{m-1/2}}{\partial x}\left\{\sum_{r=1}^{N+1}\left(a_r^m-a_r^{m-1}\right)\alpha_r^{m-1/2}\right\},\alpha_j^{m-1/2}\right\rangle_t\\
&-\left(\frac{\gamma\triangle t}{8}\right)\sum_{i=1}^{N+1} l_i^{m-1}\left\langle \alpha_i^{m-1/2}\left\{\sum_{r=1}^{N+1}\left(3k_r^{m-1}-k_r^{m-2}\right)\alpha_r^{m-1/2}\right\}^2,\alpha_j^{m-1/2}\right\rangle_t+(\gamma\triangle t)\left\langle b,\alpha_j^{m-1/2}\right\rangle_t,
\end{aligned} \tag{4.40}$$

$x\in\left[A(t_{m-1/2}),B(t_{m-1/2})\right]$, $m\in\{3,4,\ldots,M+1\}$, $j\in\{1,2,\ldots,N+1\}$.

Next we define the following vectors and matrices

$$\begin{aligned}
&\mathbf{k^m}=\left[k_1^m\,k_2^m\,\cdots k_{N+1}^m\right]^T,\quad \mathbf{l^m}=\left[l_1^m\,l_2^m\,\cdots l_{N+1}^m\right]^T,\\
&\mathbf{z_1^m}=\left[\left\langle a,\alpha_1^{m-1/2}\right\rangle_t\left\langle a,\alpha_2^{m-1/2}\right\rangle_t\cdots\left\langle a,\alpha_{N+1}^{m-1/2}\right\rangle_t\right]^T,\\
&\mathbf{z_2^m}=\left[\left\langle b,\alpha_1^{m-1/2}\right\rangle_t\left\langle b,\alpha_2^{m-1/2}\right\rangle_t\cdots\left\langle b,\alpha_{N+1}^{m-1/2}\right\rangle_t\right]^T,\\
&\left[\mathbf{A^m}\right]_{i,j}=\mathcal{A}_t\left(\alpha_i^{m-1/2},\alpha_j^{m-1/2}\right),\quad \left[\mathbf{M^m}\right]_{i,j}=\left\langle \alpha_i^{m-1/2},\alpha_j^{m-1/2}\right\rangle_t,\\
&\left[\mathbf{Q_1^m}\right]_{i,j}=\left\langle \alpha_i^{m-1/2}\left\{\sum_{r=1}^{N+1}\left(3k_r^{m-1}-k_r^{m-2}\right)\alpha_r^{m-1/2}\right\}^2,\alpha_j^{m-1/2}\right\rangle_t,\\
&\left[\mathbf{Q_2^m}\right]_{i,j}=\left\langle \frac{\partial\alpha_i^{m-1/2}}{\partial x}\left\{\sum_{r=1}^{N+1}\left(a_r^m-a_r^{m-1}\right)\alpha_r^{m-1/2}\right\},\alpha_j^{m-1/2}\right\rangle_t.
\end{aligned}$$

Using these matrices and vectors, we write equations (4.39) and (4.40) in matrix form as

$$\left[\left(1+\frac{\gamma\triangle t}{2}\right)\mathbf{M^m}+\left(\frac{\triangle t}{2}\right)\mathbf{A^m}-\left(\frac{1}{2}\right)\mathbf{Q_2^m}\right]\mathbf{k^m}=(\gamma\triangle t)\,\mathbf{z_1^m}+\left(\frac{\gamma\triangle t}{8}\right)\mathbf{Q_1^m}\left[\mathbf{l^m}+\mathbf{l^{m-1}}\right]$$
$$+\left[\left(1-\frac{\gamma\triangle t}{2}\right)\mathbf{M^m}-\left(\frac{\triangle t}{2}\right)\mathbf{A^m}+\left(\frac{1}{2}\right)\mathbf{Q_2^m}\right]\mathbf{k^{m-1}}\,, \tag{4.41}$$
$$\left[\mathbf{M^m}+\left(\frac{d\triangle t}{2}\right)\mathbf{A^m}+\left(\frac{\gamma\triangle t}{8}\right)\mathbf{Q_1^m}-\left(\frac{1}{2}\right)\mathbf{Q_2^m}\right]\mathbf{l^m}=(\gamma\triangle t)\,\mathbf{z_2^m}$$
$$+\left[\mathbf{M^m}-\left(\frac{d\triangle t}{2}\right)\mathbf{A^m}-\left(\frac{\gamma\triangle t}{8}\right)\mathbf{Q_1^m}+\left(\frac{1}{2}\right)\mathbf{Q_2^m}\right]\mathbf{l^{m-1}}\,, \tag{4.42}$$
$$m\in\{3,4,\ldots,N+1\}\,.$$

Equations (4.41) and (4.42) constitute a linear system for unknown vectors $\mathbf{k^m},\mathbf{l^m}$. Equation (4.42) should be solved first as its solution $\mathbf{l^m}$ is used to solve for $\mathbf{k^m}$ in equation (4.41). As previously noted, to solve for the fixed time t_2 vectors $\mathbf{k^2},\mathbf{l^2}$ we require a separate set of equations. Those equations are now derived.

Recall from the fixed spatial domain FEM we used a scheme to find $U^2,V^2\in\mathcal{V}_h$ that consisted of: Let $X^1=U^1$, $Y^1=V^1$. Then

$$\left\langle\frac{X^2-X^1}{\triangle t},w\right\rangle+\mathcal{A}\left(\frac{X^2+X^1}{2},w\right)=\left\langle\gamma(a-X^1+(X^1)^2Y^1),w\right\rangle\,,$$
$$\left\langle\frac{Y^2-Y^1}{\triangle t},w\right\rangle+\mathcal{A}\left(d\frac{Y^2+Y^1}{2},w\right)=\left\langle\gamma(b-(X^1)^2Y^1),w\right\rangle\,, \tag{3.27}$$
$$\left\langle\frac{U^2-U^1}{\triangle t},w\right\rangle+\mathcal{A}\left(\frac{U^2+U^1}{2},w\right)=\left\langle\gamma(a-X^{3/2}+(X^{3/2})^2Y^{3/2})),w\right\rangle\,,$$
$$\left\langle\frac{V^2-V^1}{\triangle t},w\right\rangle+\mathcal{A}\left(d\frac{V^2+V^1}{2},w\right)=\left\langle\gamma(b-(X^{3/2})^2Y^{3/2}),w\right\rangle\,, \tag{3.28}$$

where $X^{3/2}=(X^2+X^1)/(2)$, $Y^{3/2}=(Y^2+Y^1)/(2)$.

In the current context of a time dependent spatial domain we will need to modify this scheme to include the more complex basis functions and temporal derivatives, via equation (4.17), of the FEM approximations. First we let $e_i^1=k_i^1,\quad f_i^1=l_i^1,\quad i\in\{1,2,\ldots,N+1\}$. We also denote $t_2-\triangle t/2=t_{3/2}$. Then the time dependent domain equivalents of system (3.27) can be written as

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(e_i^2 - e_i^1\right)}{\triangle t} \alpha_i^{3/2} - \frac{\left(a_i^2 - a_i^1\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{e_r^2 + e_r^1}{2} \frac{\partial \alpha_r^{3/2}}{\partial x} \right) \alpha_i^{3/2} \right\}, \alpha_j^{3/2} \right\rangle_t$$
$$+ \mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{e_i^2 + e_i^1}{2} \alpha_i^{3/2}, \alpha_j^{3/2} \right) = \left\langle \gamma \left(a - \sum_{i=1}^{N+1} e_i^1 \alpha_i^{3/2} + \left(\sum_{i=1}^{N+1} e_i^1 \alpha_i^{3/2} \right)^2 \sum_{i=1}^{N+1} f_i^1 \alpha_i^{3/2} \right), \alpha_j^{3/2} \right\rangle_t ,$$
$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(f_i^2 - f_i^1\right)}{\triangle t} \alpha_i^{3/2} - \frac{\left(a_i^2 - a_i^1\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{f_r^2 + f_r^1}{2} \frac{\partial \alpha_r^{3/2}}{\partial x} \right) \alpha_i^{3/2} \right\}, \alpha_j^{3/2} \right\rangle_t$$
$$+ d\mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{f_i^2 + f_i^1}{2} \alpha_i^{3/2}, \alpha_j^{3/2} \right) = \left\langle \gamma \left(b - \left(\sum_{i=1}^{N+1} e_i^1 \alpha_i^{3/2} \right)^2 \sum_{i=1}^{N+1} f_i^1 \alpha_i^{3/2} \right), \alpha_j^{3/2} \right\rangle_t , \tag{4.43}$$
$$x \in \left[A(t_{3/2}), B(t_{3/2}) \right], j \in \{1, 2, \ldots, N+1\}.$$

Similarly, we write the time dependent domain equivalent of system (3.28) as

$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(k_i^2 - k_i^1\right)}{\triangle t} \alpha_i^{3/2} - \frac{\left(a_i^2 - a_i^1\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{k_r^2 + k_r^1}{2} \frac{\partial \alpha_r^{3/2}}{\partial x} \right) \alpha_i^{3/2} \right\}, \alpha_j^{3/2} \right\rangle_t$$
$$+ \mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{k_i^2 + k_i^1}{2} \alpha_i^{3/2}, \alpha_j^{3/2} \right) = \left\langle \gamma \left(a - \sum_{i=1}^{N+1} \left(\frac{e_i^2 + e_i^1}{2} \right) \alpha_i^{3/2} \right.\right.$$
$$\left.\left. + \left(\sum_{i=1}^{N+1} \left(\frac{e_i^2 + e_i^1}{2} \right) \alpha_i^{3/2} \right)^2 \sum_{i=1}^{N+1} \left(\frac{f_i^2 + f_i^1}{2} \right) \alpha_i^{3/2} \right), \alpha_j^{3/2} \right\rangle_t ,$$
$$\left\langle \sum_{i=1}^{N+1} \left\{ \frac{\left(l_i^2 - l_i^1\right)}{\triangle t} \alpha_i^{3/2} - \frac{\left(a_i^2 - a_i^1\right)}{\triangle t} \sum_{r=1}^{N+1} \left(\frac{l_r^2 + l_r^1}{2} \frac{\partial \alpha_r^{3/2}}{\partial x} \right) \alpha_i^{3/2} \right\}, \alpha_j^{3/2} \right\rangle_t$$
$$+ d\mathcal{A}_t \left(\sum_{i=1}^{N+1} \frac{l_i^2 + l_i^1}{2} \alpha_i^{3/2}, \alpha_j^{3/2} \right)$$
$$= \left\langle \gamma \left(b - \left(\sum_{i=1}^{N+1} \left(\frac{e_i^2 + e_i^1}{2} \right) \alpha_i^{3/2} \right)^2 \sum_{i=1}^{N+1} \left(\frac{f_i^2 + f_i^1}{2} \right) \alpha_i^{3/2} \right), \alpha_j^{3/2} \right\rangle_t . \tag{4.44}$$
$$x \in \left[A(t_{3/2}), B(t_{3/2}) \right], j \in \{1, 2, \ldots, N+1\}$$

Grouping terms of system (4.43), again using the bilinearity of the $< \cdot, \cdot >_t$ and $\mathcal{A}_t$ operations, yields

$$
\begin{aligned}
&\sum_{i=1}^{N+1} e_i^2 \left\{ \left\langle \alpha_i^{3/2}, \alpha_j^{3/2} \right\rangle_t + \left(\frac{\triangle t}{2} \right) \mathcal{A}_t \left(\alpha_i^{3/2}, \alpha_j^{3/2} \right) - \left(\frac{1}{2} \right) \left\langle \frac{\partial \alpha_i^{3/2}}{\partial x} \sum_{r=1}^{N+1} \left(a_r^2 - a_r^1 \right) \alpha_r^{3/2}, \alpha_j^{3/2} \right\rangle_t \right\} \\
&= \sum_{i=1}^{N+1} e_i^1 \left\{ (1 - \gamma \triangle t) \left\langle \alpha_i^{3/2}, \alpha_j^{3/2} \right\rangle_t - \left(\frac{\triangle t}{2} \right) \mathcal{A}_t \left(\alpha_i^{3/2}, \alpha_j^{3/2} \right) \right\} \\
&+ \sum_{i=1}^{N+1} e_i^1 \left(\frac{1}{2} \right) \left\langle \frac{\partial \alpha_i^{3/2}}{\partial x} \sum_{r=1}^{N+1} \left(a_r^2 - a_r^1 \right) \alpha_r^{3/2}, \alpha_j^{3/2} \right\rangle_t + \gamma \triangle t \left\langle a, \alpha_j^{3/2} \right\rangle_t \\
&+ (\gamma \triangle t) \sum_{i=1}^{N+1} f_i^1 \left\langle \alpha_i^{3/2} \left(\sum_{r=1}^{N+1} e_r^1 \alpha_r^{3/2} \right)^2, \alpha_j^{3/2} \right\rangle_t , \\
&\sum_{i=1}^{N+1} f_i^2 \left\{ \left\langle \alpha_i^{3/2}, \alpha_j^{3/2} \right\rangle_t + \left(\frac{d \triangle t}{2} \right) \mathcal{A}_t \left(\alpha_i^{3/2}, \alpha_j^{3/2} \right) - \left(\frac{1}{2} \right) \left\langle \frac{\partial \alpha_i^{3/2}}{\partial x} \sum_{r=1}^{N+1} \left(a_r^2 - a_r^1 \right) \alpha_r^{3/2}, \alpha_j^{3/2} \right\rangle_t \right\} \\
&= \sum_{i=1}^{N+1} f_i^1 \left\{ \left\langle \alpha_i^{3/2}, \alpha_j^{3/2} \right\rangle_t - \left(\frac{d \triangle t}{2} \right) \mathcal{A}_t \left(\alpha_i^{3/2}, \alpha_j^{3/2} \right) \right\} \\
&+ \sum_{i=1}^{N+1} f_i^1 \left(\frac{1}{2} \right) \left\langle \frac{\partial \alpha_i^{3/2}}{\partial x} \sum_{r=1}^{N+1} \left(a_r^2 - a_r^1 \right) \alpha_r^{3/2}, \alpha_j^{3/2} \right\rangle_t + \gamma \triangle t \left\langle b, \alpha_j^{3/2} \right\rangle_t \\
&- (\gamma \triangle t) \sum_{i=1}^{N+1} f_i^1 \left\langle \alpha_i^{3/2} \left(\sum_{r=1}^{N+1} e_r^1 \alpha_r^{3/2} \right)^2, \alpha_j^{3/2} \right\rangle_t , \qquad (4.45) \\
&x \in \left[A(t_{3/2}), B(t_{3/2}) \right] , j \in \{1, 2, \ldots, N+1\} .
\end{aligned}
$$

In order to write (4.45) in matrix form we denote the following matrices and vectors

$$
\begin{aligned}
&\mathbf{e^2} = \left[e_1^2 \, e_2^2 \cdots e_{N+1}^2 \right]^T , \quad \mathbf{f^2} = \left[f_1^2 \, f_2^2 \cdots f_{N+1}^2 \right]^T , \\
&\mathbf{e^1} = \left[e_1^1 \, e_2^1 \cdots e_{N+1}^1 \right]^T , \quad \mathbf{f^1} = \left[f_1^1 \, f_2^1 \cdots f_{N+1}^1 \right]^T , \\
&\mathbf{z_3} = \left[\left\langle a, \alpha_1^{3/2} \right\rangle_t \left\langle a, \alpha_2^{3/2} \right\rangle_t \cdots \left\langle a, \alpha_{N+1}^{3/2} \right\rangle_t \right]^T , \\
&\mathbf{z_4} = \left[\left\langle b, \alpha_1^{3/2} \right\rangle_t \left\langle b, \alpha_2^{3/2} \right\rangle_t \cdots \left\langle b, \alpha_{N+1}^{3/2} \right\rangle_t \right]^T , \\
&\left[\mathbf{A_2} \right]_{i,j} = \mathcal{A}_t \left(\alpha_i^{3/2}, \alpha_j^{3/2} \right) , \quad \left[\mathbf{M_2} \right]_{i,j} = \left\langle \alpha_i^{3/2}, \alpha_j^{3/2} \right\rangle_t , \\
&\left[\mathbf{Q_3} \right]_{i,j} = \left\langle \alpha_i^{3/2} \left\{ \sum_{r=1}^{N+1} e_r^1 \alpha_r^{3/2} \right\}^2, \alpha_j^{3/2} \right\rangle_t , \\
&\left[\mathbf{Q_4} \right]_{i,j} = \left\langle \frac{\partial \alpha_i^{3/2}}{\partial x} \left\{ \sum_{r=1}^{N+1} \left(a_r^2 - a_r^1 \right) \alpha_r^{3/2} \right\}, \alpha_j^{3/2} \right\rangle_t .
\end{aligned}
$$

Using these matrices and vectors, we can write system (4.45) as

$$
\begin{aligned}
&\left[\mathbf{M_2}+\left(\frac{\triangle t}{2}\right)\mathbf{A_2}-\left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{e^2}\\
&=\left[(1-\gamma\triangle t)\,\mathbf{M_2}-\left(\frac{\triangle t}{2}\right)\mathbf{A_2}+\left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{e^1}+(\gamma\triangle t)\left[\mathbf{z_3}+\mathbf{Q_3}\mathbf{f^1}\right],\\
&\left[\mathbf{M_2}+\left(\frac{d\triangle t}{2}\right)\mathbf{A_2}-\left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{f^2}\\
&=\left[\mathbf{M_2}-\left(\frac{d\triangle t}{2}\right)\mathbf{A_2}+\left(\frac{1}{2}\right)\mathbf{Q_4}-(\gamma\triangle t)\,\mathbf{Q_3}\right]\mathbf{f^1}+(\gamma\triangle t)\,\mathbf{z_4}\,. \qquad (4.46)
\end{aligned}
$$

System (4.46) yields the solution vectors $\mathbf{e^2},\mathbf{f^2}$ to be used in system (4.44). System (4.44) written in grouped form is

$$
\begin{aligned}
&\sum_{i=1}^{N+1}k_i^2\left\{\left\langle\alpha_i^{3/2},\alpha_j^{3/2}\right\rangle_t+\left(\frac{\triangle t}{2}\right)\mathcal{A}_t\left(\alpha_i^{3/2},\alpha_j^{3/2}\right)-\left(\frac{1}{2}\right)\left\langle\frac{\partial\alpha_i^{3/2}}{\partial x}\sum_{r=1}^{N+1}\left(a_r^2-a_r^1\right)\alpha_r^{3/2},\alpha_j^{3/2}\right\rangle_t\right\}\\
&=\sum_{i=1}^{N+1}k_i^1\left\{\left\langle\alpha_i^{3/2},\alpha_j^{3/2}\right\rangle_t-\left(\frac{\triangle t}{2}\right)\mathcal{A}_t\left(\alpha_i^{3/2},\alpha_j^{3/2}\right)+\left(\frac{1}{2}\right)\left\langle\frac{\partial\alpha_i^{3/2}}{\partial x}\sum_{r=1}^{N+1}\left(a_r^2-a_r^1\right)\alpha_r^{3/2},\alpha_j^{3/2}\right\rangle_t\right\}\\
&+(\gamma\triangle t)\left\{\left\langle a,\alpha_j^{3/2}\right\rangle_t-\sum_{i=1}^{N+1}\left(\frac{e_i^2+e_i^1}{2}\right)\left\langle\alpha_i^{3/2},\alpha_j^{3/2}\right\rangle_t\right.\\
&\left.+\sum_{i=1}^{N+1}\left(\frac{f_i^2+f_i^1}{2}\right)\left\langle\alpha_i^{3/2}\left(\sum_{r=1}^{N+1}\left(\frac{e_r^2+e_r^1}{2}\right)\alpha_r^{3/2}\right)^2,\alpha_j^{3/2}\right\rangle_t\right\},\\
&\sum_{i=1}^{N+1}l_i^2\left\{\left\langle\alpha_i^{3/2},\alpha_j^{3/2}\right\rangle_t+\left(\frac{d\triangle t}{2}\right)\mathcal{A}_t\left(\alpha_i^{3/2},\alpha_j^{3/2}\right)-\left(\frac{1}{2}\right)\left\langle\frac{\partial\alpha_i^{3/2}}{\partial x}\sum_{r=1}^{N+1}\left(a_r^2-a_r^1\right)\alpha_r^{3/2},\alpha_j^{3/2}\right\rangle_t\right\}\\
&=\sum_{i=1}^{N+1}l_i^1\left\{\left\langle\alpha_i^{3/2},\alpha_j^{3/2}\right\rangle_t-\left(\frac{d\triangle t}{2}\right)\mathcal{A}_t\left(\alpha_i^{3/2},\alpha_j^{3/2}\right)+\left(\frac{1}{2}\right)\left\langle\frac{\partial\alpha_i^{3/2}}{\partial x}\sum_{r=1}^{N+1}\left(a_r^2-a_r^1\right)\alpha_r^{3/2},\alpha_j^{3/2}\right\rangle_t\right\}\\
&+(\gamma\triangle t)\left\{\left\langle b,\alpha_j^{3/2}\right\rangle_t-\sum_{i=1}^{N+1}\left(\frac{f_i^2+f_i^1}{2}\right)\left\langle\alpha_i^{3/2}\left(\sum_{r=1}^{N+1}\left(\frac{e_r^2+e_r^1}{2}\right)\alpha_r^{3/2}\right)^2,\alpha_j^{3/2}\right\rangle_t\right\}, \qquad (4.47)\\
&x\in\left[A(t_{3/2}),B(t_{3/2})\right],j\in\{1,2,\ldots,N+1\}\,.
\end{aligned}
$$

In order to write (4.47) in matrix form we denote

$$
\begin{aligned}
&\mathbf{k^2} = \left[k_1^2\, k_2^2 \cdots k_{N+1}^2\right]^T, \quad \mathbf{l^2} = \left[l_1^2\, l_2^2 \cdots l_{N+1}^2\right]^T, \\
&\mathbf{z_3} = \left[\left\langle a, \alpha_1^{3/2}\right\rangle_t \left\langle a, \alpha_2^{3/2}\right\rangle_t \cdots \left\langle a, \alpha_{N+1}^{3/2}\right\rangle_t\right]^T, \\
&\mathbf{z_4} = \left[\left\langle b, \alpha_1^{3/2}\right\rangle_t \left\langle b, \alpha_2^{3/2}\right\rangle_t \cdots \left\langle b, \alpha_{N+1}^{3/2}\right\rangle_t\right]^T, \\
&[\mathbf{A_2}]_{i,j} = \mathcal{A}_t\left(\alpha_i^{3/2}, \alpha_j^{3/2}\right), \quad [\mathbf{M_2}]_{i,j} = \left\langle \alpha_i^{3/2}, \alpha_j^{3/2}\right\rangle_t, \\
&[\mathbf{Q_4}]_{i,j} = \left\langle \frac{\partial \alpha_i^{3/2}}{\partial x}\left\{\sum_{r=1}^{N+1}\left(a_r^2 - a_r^1\right)\alpha_r^{3/2}\right\}, \alpha_j^{3/2}\right\rangle_t, \\
&[\mathbf{Q_5}]_{i,j} = \left\langle \alpha_i^{3/2}\left\{\sum_{r=1}^{N+1}\left(\frac{e_r^2 + e_r^1}{2}\right)\alpha_r^{3/2}\right\}^2, \alpha_j^{3/2}\right\rangle_t.
\end{aligned}
$$

Using these matrices and vectors, we write system (4.47) as

$$
\begin{aligned}
&\left[\mathbf{M_2} + \left(\frac{\triangle t}{2}\right)\mathbf{A_2} - \left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{k^2} \\
&= \left[\mathbf{M_2} - \left(\frac{\triangle t}{2}\right)\mathbf{A_2} + \left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{k^1} + (\gamma \triangle t)\left[\mathbf{z_3} - \mathbf{M_2}\left(\frac{\mathbf{e^2} + \mathbf{e^1}}{2}\right) + \mathbf{Q_5}\left(\frac{\mathbf{f^2} + \mathbf{f^1}}{2}\right)\right], \\
&\left[\mathbf{M_2} + \left(\frac{d\triangle t}{2}\right)\mathbf{A_2} - \left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{l^2} \\
&= \left[\mathbf{M_2} - \left(\frac{d\triangle t}{2}\right)\mathbf{A_2} + \left(\frac{1}{2}\right)\mathbf{Q_4}\right]\mathbf{l^1} + (\gamma \triangle t)\left[\mathbf{z_4} + \mathbf{Q_5}\left(\frac{\mathbf{f^2} + \mathbf{f^1}}{2}\right)\right].
\end{aligned} \tag{4.48}
$$

System (4.48) yields the solution vectors $\mathbf{k^2}, \mathbf{l^2}$ that in conjunction with $\mathbf{k^1}, \mathbf{l^1}$ from initial conditions serve to solve the general equations (4.41) and (4.42). For this Crank-Nicolson discretization and the previous Backward Euler discretization an algorithm was written to model pattern formation. The results of this algorithm are presented next.

4.4 Computational Results

Algorithm results for the time dependent spatial domain are presented in this section. We note that for this algorithm we have prescribed simple linear growth of the spatial domain. For application to specific biological systems we would desire more intricate models of growth [8]. However, in studying the use of efficient computational models, linear growth is sufficient.

We notice that pattern formation on a growing domain shows that a single pattern is not formed and then maintained in time. Rather, patterns tend to form and then change to a new pattern as time increases. In Figures 4.1 and 4.2 we show a pattern modeled on a linearly growing domain for Schnakenberg kinetics using parameters $a = 0.1$, $b = 0.9$, $d = 10$, $\gamma = 25$.

Specifically, we observe an increase in the wavelength of patterns produced as the spatial domain

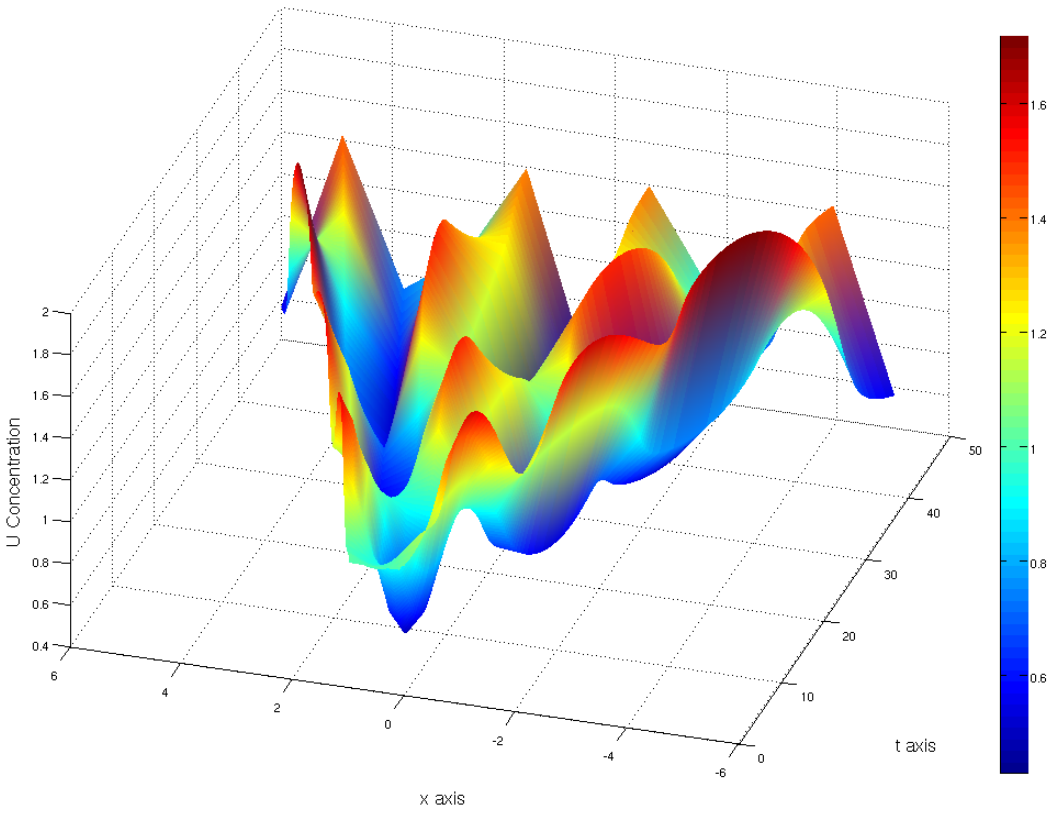


Figure 4.1: Time Dependent Domain Pattern Formation

grows. We believe that this is observed due to the non-dimensionalization we conducted in Chapter 2. Recall that for Schnakenberg kinetics we defined the parameter γ:

$$\gamma = \frac{k_2 L_x^2}{d_1}$$

Thus when domain growth occurs we are in effect changing γ as well. In Figure 4.2 we observe a 2π pattern for $t \approx 7.5$, $x \in (-0.5, 1.5)$. As $\gamma = 25$ was used in this figure we conclude is was in effect acting as $\gamma = 100$ at this time. A 2π pattern for $\gamma = 100$ is consistent with the predicted parameter space and mode excitation from Table 2.1. We also observe for $t \approx 20$, $x \in (-2, 3)$ a 4π pattern. We would expect that γ was in effect acting as $\gamma = 625$ here. Table 2.1 predicts a 4π pattern for this value. Hence the algorithm is displaying effects as predicted. This serves as a validation of our simulation.

Similar to the mode isolation tests conducted on the fixed domain, we have varied the γ parameter to see how this effects pattern formation in the moving domain simulations. Figures 4.3 and 4.4 respectively show Backward Euler moving FEM runs with $\gamma = 85$ and $\gamma = 200$. The other

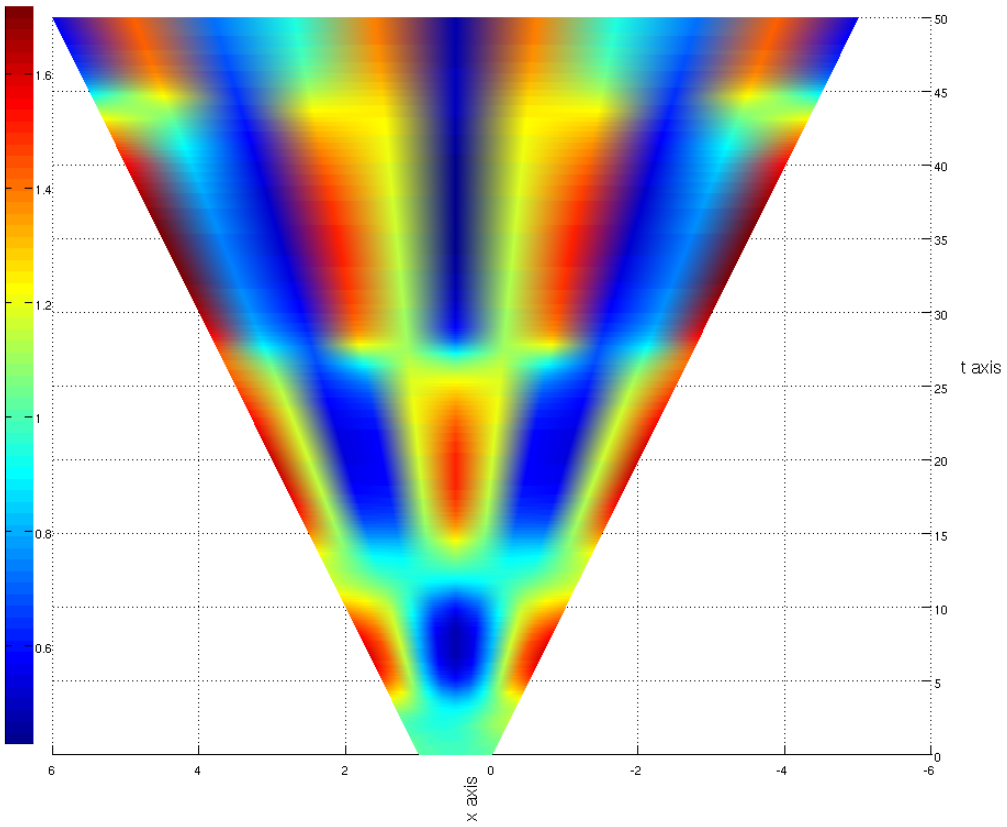


Figure 4.2: Time Dependent Domain Pattern Formation, Top View

parameters were fixed as $a = 0.1$, $b = 0.9$, $d = 10$.

Figures 4.4 and 4.5 respectively show Crank-Nicolson moving FEM runs with $\gamma = 85$ and $\gamma = 200$. The other parameters were fixed as $a = 0.1$, $b = 0.9$, $d = 10$.

In Figures 4.3-4.6 we observe that these simulations show the expected increase in wavelengths due to manipulation of the parameter γ.

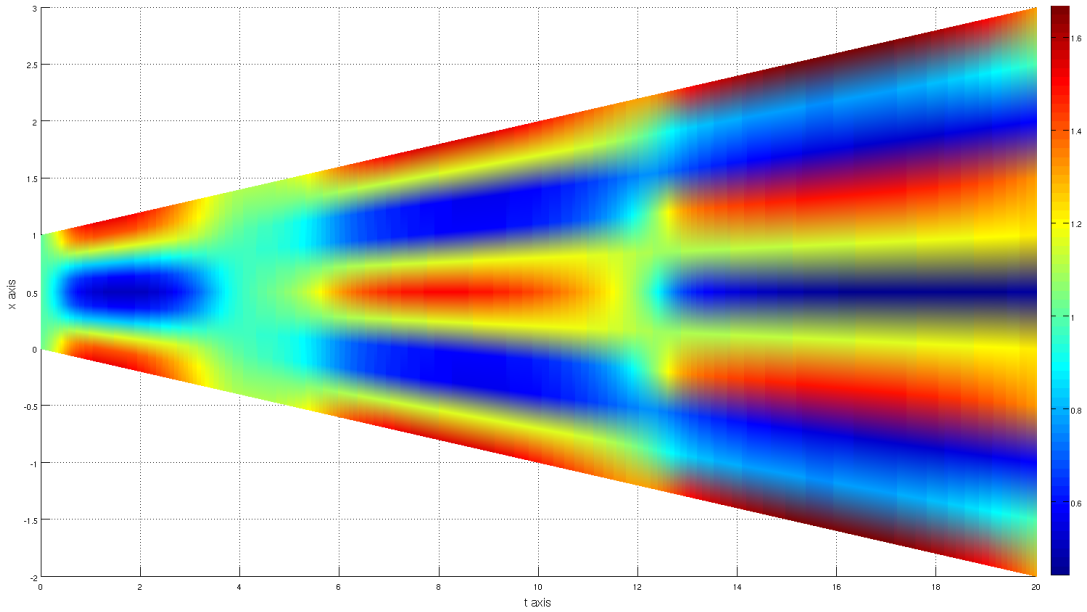


Figure 4.3: Backwards Euler, Schnakenberg,$\gamma = 85$, Top View

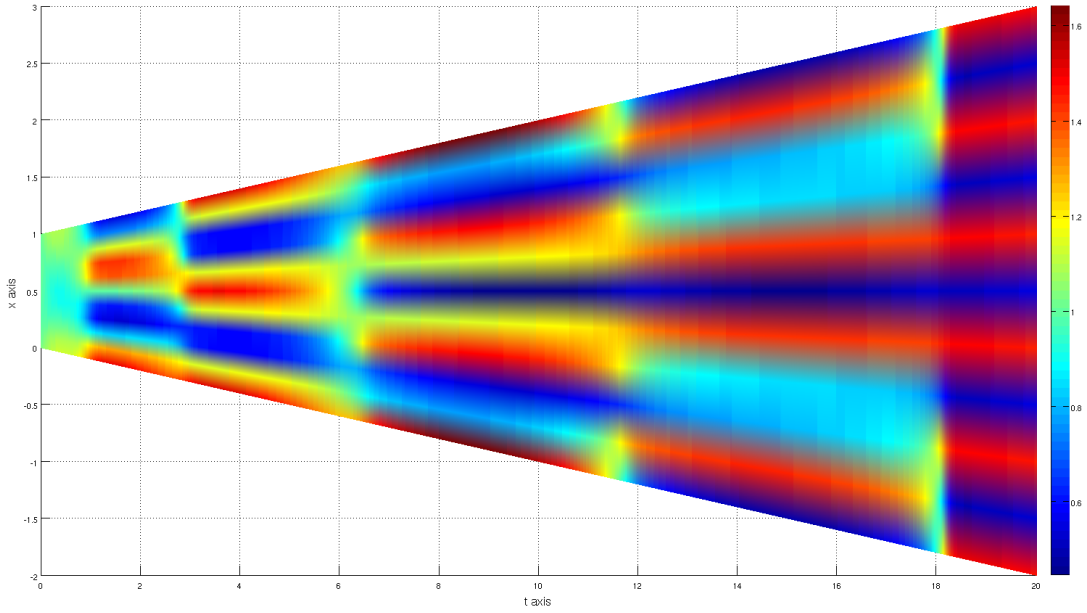


Figure 4.4: Backwards Euler, Schnakenberg,$\gamma = 200$, Top View

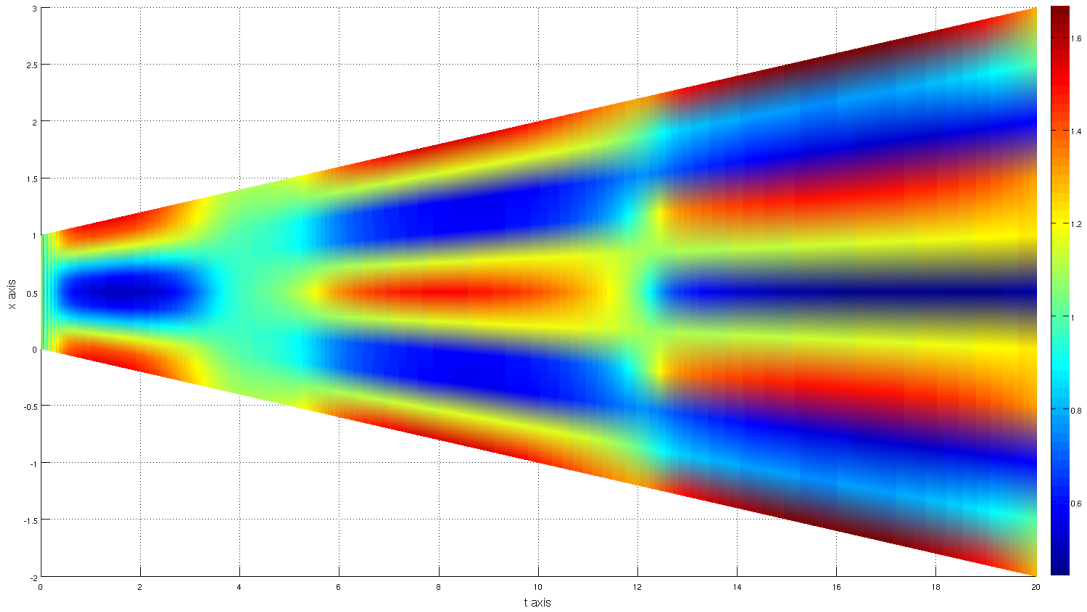


Figure 4.5: Crank-Nicolson, Schnakenberg,$\gamma = 85$, Top View

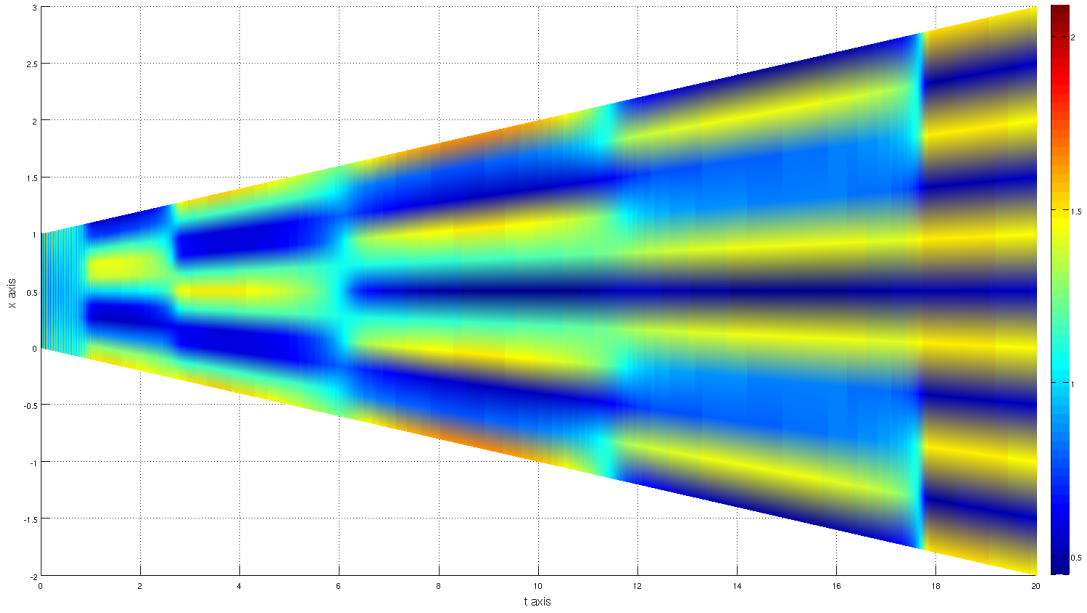


Figure 4.6: Crank-Nicolson, Schnakenberg,$\gamma = 200$, Top View

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

In this thesis we developed and demonstrated efficient computational pattern formation models. These models show pronounced reduction in computational time to simulate pattern formation on stationary and evolving domains. This improvement becomes more useful for long time simulations. Specifically, in cases where run-times are expected to be on the order of days, the higher efficiency model is exceptionally useful to realize pattern formation on moving domains with various parameters.

Future work on our computational models could yield simulation on higher dimensional spatial domains. Expansion of the formulation to two dimensional and three dimensional spatial domains would be exceptionally interesting, as this could expand the applications of this algorithm greatly. In general, the discretization and linearization have performed exceptionally for all of our simulations. Efficient implementation of our schemes will facilitate much improved future pattern formation models.

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