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Dynamics of Activator Inhibitor Reaction-Diffusion Systems

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ABSTRACT

This thesis seeks primarily to contribute to an attempt to understand the patterns we see in nature, such as pigmentation in animals, branching in trees and skeletal structures, as well as how the vast range of patterns and structures emerge from an almost uniformly homogeneous fertilized egg, through survey and study as well as improve a number of mathematical models of reaction-diffusion of the type activator-inhibitor and related systems. The main objective is to conduct mathematical analysis and numerical simulations of the such models under two different effects, the first one, is time-fractional derivative instead of classical derivative; Where we have established algebraic conditions for the asymptotic stability of time-fractional reaction-diffusion systems in these cases, commensurate/incommensurate and linear/nonlinear. We have also presented in this context, new predictor-corrector numerical schemes suitable for fractional differential equations with/without delay and time-fractional reaction-diffusion systems. Numerical formulas are presented that approximate the Caputo as well as Caputo-Fabrizio and Atangana-Baleanu fractional derivatives. In addition, a case study is considered where the proposed schemes is used to obtain numerical solutions of the Gierer-Meinhardt activator-inhibitor model with the aim of assessing the system's dynamics. The second one, is the effects of growth of spatial domain, evolving of domains was incorporated into activator-inhibitor reaction-diffusion systems and others then the existence as well as the asymptotic behavior of solutions is proved under certain conditions using Lyapunov functionals combined with the regularization effect of the parabolic equation. To confirm and validate the analytical results, numerical simulations are employed.

Keywords Reaction-diffusion, activator-inhibitor models, existence of solutions, asymptotic stability, fractional calculus, evolving domains.

Résumé

Cette thèse vise principalement à contribuer à une tentative de comprendre les modèles que nous voyons dans la nature, tels que la pigmentation chez les animaux, la ramification des arbres et les structures squelettiques, ainsi que la façon dont une grande variété de modèles et de structures émergent d'un œuf fécondé presque homogène, par le biais d'enquêtes et d'études ainsi que l'amélioration d'un certain nombre de modèles mathématiques des systèmes réaction-diffusion de type activateur-inhibiteur et des systèmes associés. L'objectif principal est d'effectuer l'analyse mathématique et la simulation numérique de ces modèles sous deux influences différentes, la première est la dérivée fractionnaire au lieu de la dérivée classique par rapport au temps ; Où l'on établit des conditions algébriques pour la stabilité asymptotique des systèmes de réaction-diffusion dans ces cas, équivalentes/non-équivalentes et linéaires/non-linéaires. Nous avons également présenté dans ce contexte, de nouveaux schémas numériques à prédiction-corrigée adaptés aux équations différentielles fractionnaires avec/sans retard et aux systèmes de réaction-diffusion incorporant la dérivée fractionnaire par rapport au temps. Des formules numériques sont présentées qui ciblent plusieurs types de dérivés fractionnaires, y compris Caputo ainsi que les dérivés Caputo-Fabrizio et Atangana-Baleanu. De plus, une étude de cas particulière est considérée où les schémas proposés sont utilisés pour obtenir des solutions numériques du modèle activateur-inhibiteur de Gierer-Meinhardt dans le but d'évaluer la dynamique du système. Le second, ce sont les effets de la croissance du domaine spatial, et l'évolution des domaines a été incorporée dans les systèmes de réaction-diffusion de type activateur-inhibiteur et autres, où l'existence des solutions globales et leur comportement asymptotique sous certaines conditions ont été démontrées à l'aide des fonctions de Lyapunov ainsi que l'effet de régularisation d'équation parabolique. Pour confirmer et valider les résultats analytiques, des simulations numériques sont utilisées.

Mots-clés: Réaction-diffusion, modèles activateur-inhibiteur, existence des solutions, stabilité asymptotique, calcul fractionnaire, domaines évolutifs.

ملخص

تسعى هذه الأطروحة في المقام الأول إلى المساهمة في محاولة فهم الأنماط التي نراها في الطبيعة، مثل التصبغ في الحيوانات، والتفرع في الأشجار والكيانات الهيكلية، وكذلك كيفية ظهور مجموعة واسعة من الأنماط والهياكل من بيضة مخضبة متجانسة تقريبًا، من خلال مسح ودراسة وكذلك تحسين عدد من النماذج الرياضية الخاصة بأنظمة التفاعل-الانتشار من نوع منشط-مضطرب والأنظمة ذات الصلة. الهدف الرئيسي هو إجراء التحليل الرياضي ومحاكاة عددية لهذه النماذج تحت تأثيرين مختلفين، التأثير الأول يتمثل في المشتق كسري بدلاً من المشتق الكلاسيكي بالنسبة للزمن؛ حيث تم وضع شروط جبرية للاستقرار المقارب لأنظمة التفاعل-الانتشار في هذه الحالات، متكافئة غير متكافئة وخطية غير خطية. تم أيضًا في هذا السياق اقتراح مخططات رقمية جديدة للتنبؤ-المصحح مناسبة للمعادلات التفاضلية الكسرية مع إبدون تأخير وأنظمة التفاعل-الانتشار التي تتضمن المشتق الكسري بالنسبة للزمن. يتم تقديم الصيغ العددية التي تستهدف عدة أنواع من المشتقات الكسرية نذكر منها Caputo وكذلك مشتقات Caputo-Fabrizio و Atangana-Baleanu بالإضافة إلى ذلك، يتم النظر في دراسة حالة خاصة حيث يتم استخدام المخططات المقترحة للحصول على حلول عددية لنموذج منشط-مضطرب Gierer-Meinhardt بهدف تقييم ديناميكيات النظام. والتأثير الثاني، يتمثل في آثار نمو المجال المكاني، حيث تم دمج تطور المجالات في أنظمة التفاعل-الانتشار من نوع منشط-مضطرب وغيرها، فقد تم إثبات وجود الحلول الأبدية وسلوكها المقارب في ظل ظروف معينة باستخدام وظائف Lyapunov جنبًا إلى جنب مع تأثير فعل الصاقلة للمعادلات التفاضلية الجزئية من نوع القطع المكافئ. لتأكيد والتحقق من صحة النتائج التحليلية يتم استخدام المحاكاة العددية.

كلمات مفتاحية: تفاعل-انتشار، نماذج منشط-مضطرب، وجود الحلول، الاستقرار المقارب، التفاضل والتكامل الكسري، المجالات المتطورة.

LIST OF NOTATIONS

<i>Symbol/Notaion</i>	<i>Descreption</i>
\mathbb{N} or \mathbb{Z}^+	The set of all positive integers: $1, 2, \dots$
\mathbb{N}_0	$\mathbb{N} \cup \{0\}$
\mathbb{R}	The set of real numbers
\mathbb{R}_+	The set of all nonnegative real numbers
\mathbb{R}_+^*	The set of all positive real numbers
\mathbb{R}^N	The set of all N-tuples $x = (x_1, x_2, \dots, x_N)$
$x^T \in \mathbb{R}^N$	The transpose of vector $x \in \mathbb{R}^N$
Ω	An open bounded subset of \mathbb{R}^N
\mathbb{C}	The set of complex numbers
$f \star g$	Convolution product of functions f and g
<i>l.c.m</i>	Least common multiple

<i>Symbol/Notaion</i>	<i>Descreption</i>
$g.c.d$	Greatest common divisor
$D(A)$	The Domain of an operator A
M^{-1}	The inverse of a matrix M
$\text{Tr}(M)$	The trace of a matrix M
$\det(M)$	The determinant of a matrix M
M^T	The transpose of a matrix M
$\text{Re}(z)$	The real part of a complex number z
$\arg(z)$	The argument of a complex number z
$\frac{\partial g(x_1, \dots, x_N)}{\partial x_k}$	The partial derivative of $g: \mathbb{R}^N \rightarrow \mathbb{R}$ with respect to x_k
$\nabla g := \left(\frac{\partial g}{\partial x_1}, \dots, \frac{\partial g}{\partial x_N} \right)$	The Nabla operator of a function $g: \mathbb{R}^N \rightarrow \mathbb{R}$
$\Delta g = \sum_{k=1}^N \frac{\partial^2}{\partial x_k^2} g$	The Laplacian of a function $g: \mathbb{R}^N \rightarrow \mathbb{R}$
$C(\Omega)$	The space of continuous functions on Ω
$C^k(\Omega), k \in \mathbb{N}$	The space of continuously k -differentiable functions on Ω
$L^p(\Omega)$	Lebesgue spaces (where, $1 \leq p \leq \infty$) on Ω
$W^{k,p}(\Omega)$	Sobolev space (where, $1 \leq p \leq \infty, k \in \mathbb{N}_0$) on Ω
$H^k(\Omega)$	Sobolev space (where, $p = 2, k \in \mathbb{N}_0$) on Ω
$[\mathcal{X}]^m$	The multiplication m -times of Banach space \mathcal{X} .

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INTRODUCTION

In many real-world systems, explaining how spatial patterns emerges from homogeneity as well as spread of epidemics (see Figure 1 and Figure 2) are key questions.

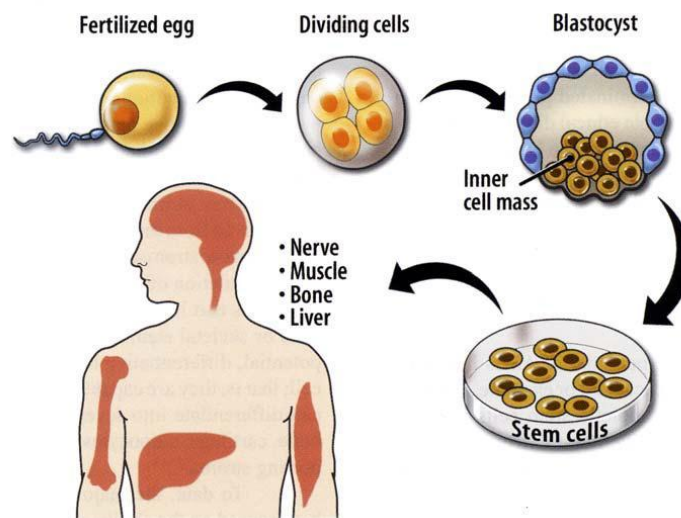


Figure 1: From a fertilized egg (almost homogeneous) to an elegant body (cf. [99]).

With the beginning of the fifties of the last century Alan Turing provide a sophisticated explanation for this phenomenon through his pioneering scientific paper (cf. [104]) entitled: "The chemical basis of morphogenesis". Turing proposed that the patterns we see during embryonic development are caused by morphogens, which are biochemicals

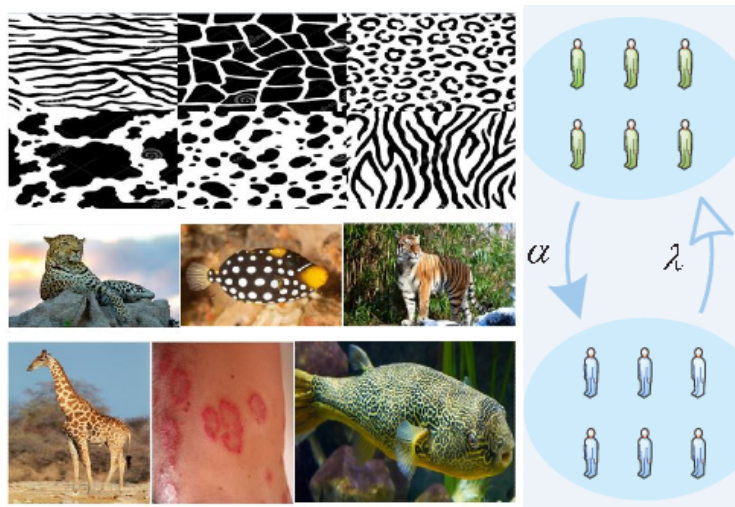


Figure 2: Patterns in living things pigmentation as well as transmission of epidemics.

that have a spatial pre-pattern. Cells would then differentiate in a threshold-dependent manner in response to this pre-pattern, precisely, the reason behind these patterns is diffusion-driven instability in reaction-diffusion system (cf. [73, 74, 83]). This means that an ODE system that is asymptotically stable but becomes unstable with the inclusion of the Laplacian denoting spatial diffusion. Since then, this elegant idea has received great attention from the research community in the fields of mathematics, biology, chemistry and many more. Depending on the signs of the Jacobian matrix considered as the approximation of nonlinearities (reaction kinetics) at the the equilibrium point of model, these Turing systems can be classified into two main types: activator-inhibitor and positive feedback. In this thesis, we are interested in activator-inhibitor systems. At least case with two interacting substances, this means that one of the substances acts as an activator enforcing the formation of itself along with the second substance. On the other hand, the second substance acts as an inhibitor preventing the formation of both substances. Such systems include the well-known Gierer-Meinhardt system [2, 42], the Lengyel-Epstein system [1, 57], the Brusselator system [87], and the Schnakenberg system [97]. This thesis is divided in four chapters, as follows:

Chapter 1: In this chapter, we provide some of the basic terminology as well as some preliminary definitions for fractional calculus, semigroup theory, unbounded operators, and formulas that will be important in the next chapters.

Chapter 2: Our aim in this chapter is to establish sufficient conditions for the asymptotic stability of generic time-fractional reaction-diffusion systems, which to the best of the authors' knowledge has not been investigated wholly in the literature. We present

the derived stability criteria for commensurate and incommensurate, linear time-fractional reaction-diffusion systems, as well as we deal with the stability of nonlinear systems. In addition, two numerical examples with different parameter sets are presented to illustrate the derived theoretical conditions.

Chapter 3: This chapter is divided in three sections. In the first section, we have employed two/three step first/second order Newton polynomial interpolation to derive two new methods suitable for solving fractional differential equations with several definitions of the fractional derivative. The first method is an improved version of the Newton interpolation based Atangana–Seda scheme, which has attracted the attention of several researchers in the short time since its appearance. In our improved version, we take into account previously neglected terms and show that the corresponding performance improvement is worth the effort. The second proposed method is of the predictor corrector type which uses the improved Atangana–Seda scheme as the predictor step. Numerical formulas are derived based on the new methods for three different types of derivatives, namely: the Caputo, Caputo–Fabrizio, and Atangana-Baleanu fractional derivatives. The effectiveness of the proposed methods is demonstrated by means of various numerical examples in which we attempt to obtain accurate approximate solutions for complex systems. In these worked examples, we start with some simple single equations extracted from the literature and end with the well established realistic Gierer-Meinhardt model describing the morphogenesis process. In the second section, we derived a numerical approximation to the variable-order fractional delay differential equations with multiple lags, based on Adams-Bashforth-Moulton method. The detailed error analysis of the numerical method was studied under a specific condition on the non linear term. Numerical examples showed the efficiency of the suggested scheme. In the third section, we propose a numerical method for solving time fractional order reaction-diffusion system. The numerical method are obtained considering the Method of Lines (MOL) approach, the partial derivatives with respect to the spatial variables are discretized to obtain a system of ODEs with respect to the time variable and then our schemes and then our schemes mentioned in the previous sections in the current chapter can be used to solve this fractional differential systems. This method is compared with the finite difference method applied to a specific time-fractional Schnakenberg-reaction-diffusion model.

Chapter 4: This chapter is divided in three sections. In the first section, we give a positive answer to the open question about the global existence, uniqueness and uniform boundedness of solution of Gierer-Meinhardt system on a class of spatially linear isotropically evolving domain. In the second section, we prove the global existence, uniqueness and uniform boundedness of solutions for a class of weakly coupled reaction-diffusion systems on domains with unbounded growth, and nonlinearities of exponential

growth. We will also show that under certain conditions on growth of domain, we get the global asymptotic stability of such systems. To our best knowledge, this results seems to be the first attempt to consider the nonlinearities of exponential growth in reaction-diffusion systems on the time varying domains. In the third section, we present a uniform boundedness of solutions for reaction-diffusion systems thus the existence of global solutions on isotropic time-dependent domains and reaction functions are growing faster than an exponential function respect to the second unknown function. Moreover, we exhibit on a class of time-dependent spatial domains, the global stability of trivial solution of the proposed systems.

CHAPTER

1

PRELIMINARIES AND BACKGROUND

This chapter collects some fundamental results and notations that will be utilized throughout this thesis.

This chapter is divided into four sections: In the first section, we review several fundamental concepts of fractional calculus. In the second section, we mention some basic concepts of semigroups and present their most important properties that will be used later. In the second section, we outline the basic steps for obtaining a mathematical model of real phenomena, more specifically when the latter includes systems composed of chemical compounds, population density, ... etc, where the sub-sections will respectively assign the modeling of biochemical, population phenomena, ... etc, in a fixed bounded domain evolved bounded domain. In the fourth part, we provide the most important known results concerning the local and global existence and uniqueness of classical solutions of reaction-diffusion systems as well as comparison principle.

1.1 Fractional calculus

Throughout this section, we have relied on several references (see e.g. [51, 59, 60, 61, 69, 70, 86, 95, 96]).

1.1.1 Some useful special functions for fractional calculus

In this part, we present two main functions for fractional calculus. We define Euler's Gamma function and Beta function, then we introduce some properties related to these functions.

Gamma function

Definition 1.1.1. Let $\alpha > 0$, the Gamma function $\Gamma(\alpha)$ is defined by the following Euler integral:

$$\Gamma(\alpha) = \int_0^{+\infty} e^{-s} s^{\alpha-1} ds. \quad (1.1)$$

It is clear that the Gamma function is well-defined through the convergence of integral (1.1). In the following, we collect the most important properties of the Gamma function:

Proposition 1.1.1. Let $\alpha > 0$, we have

1. $\Gamma(\alpha) > 0$.
2. The Gamma function $\Gamma(\alpha)$ is continuous.
3. $\Gamma(\alpha + 1) = \alpha\Gamma(\alpha)$.
4. $\Gamma(n + 1) = n!$, for all $n \in \mathbb{N}_0$.

Beta function

Definition 1.1.2. Let $\alpha, \beta > 0$, the Beta function $B(\alpha, \beta)$ is defined by the following integral:

$$B(\alpha, \beta) = \int_0^1 s^{\alpha-1} (1-s)^{\beta-1} ds. \quad (1.2)$$

In the following, we enumerate the most important properties of the Beta function:

Proposition 1.1.2. Let $\alpha, \beta > 0$, we have

1. $B(\alpha, \beta) = B(\beta, \alpha)$.
2. $B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$ (where $\Gamma(\cdot)$ is the Gamma function).
3. $B(\alpha, \beta) = \frac{\beta-1}{\alpha+\beta-1} B(\alpha, \beta-1)$, for all $\beta > 1$.

1.1.2 Fractional integrals

Definition 1.1.3. The left-sided α -order Riemann–Liouville fractional integral of a function $f(t)$ is defined as

$${}_0I_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} f(s) ds, \quad (1.3)$$

where $\alpha > 0$.

Definition 1.1.4. Let $f \in C([0, T])$, $\alpha(t) > 0$, and $T > 0$, the left-sided Riemann–Liouville variable-order integral is defined as follows:

$${}_0I_t^{\alpha(t)} f(t) = \frac{1}{\Gamma(\alpha(t))} \int_0^t (t-\eta)^{\alpha(t)-1} f(\eta) d\eta, \quad t > 0. \quad (1.4)$$

Definition 1.1.5. The left-sided Caputo–Fabrizio fractional integral of a function $f(t)$ is defined as

$${}_0^{CF}I_t^\alpha f(t) = \frac{1-\alpha}{M(\alpha)} f(t) + \frac{\alpha}{M(\alpha)} \int_0^t f(s) ds, \quad (1.5)$$

where $\alpha \in (0, 1)$, and $M(\alpha)$ is a normalization function satisfying $M(0) = M(1) = 1$.

Definition 1.1.6. The left-sided Atangana-Baleanu fractional integral of a function $f(t)$ is defined as

$${}_{0}^{\text{AB}}\Gamma_t^\alpha f(t) = \frac{1-\alpha}{\text{AB}(\alpha)} f(t) + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \int_0^t f(s) (t-s)^{\alpha-1} ds, \quad (1.6)$$

where $\alpha \in (0, 1)$, and

$$\text{AB}(\alpha) = 1 - \alpha + \frac{\alpha}{\Gamma(\alpha)}. \quad (1.7)$$

Definition 1.1.7. The convolution kernel of order $\alpha > 0$ for fractional integrals is denoted by $Y_\alpha(t)$ and defined as

$$Y_\alpha(t) := \frac{t_+^{\alpha-1}}{\Gamma(\alpha)} \in L_{loc}^1(\mathbb{R}_+^*),$$

where

$$t_+^{\alpha-1} = \begin{cases} t^{\alpha-1} & \text{if } t > 0, \\ 0 & \text{if } t \leq 0. \end{cases}$$

Remark 1.1.1. Y_α has convolution property (i.e. $Y_\alpha \star Y_\beta \equiv Y_{\alpha+\beta}$, for all $\alpha, \beta > 0$), indeed

$$\begin{aligned} (Y_\alpha \star Y_\beta)(t) &= \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_0^t (t-\tau)^{\alpha-1} \tau^{\beta-1} d\tau \\ &= \frac{\text{B}(\alpha, \beta)}{\Gamma(\alpha)\Gamma(\beta)} t_+^{\alpha+\beta-1} \\ &= \frac{1}{\Gamma(\alpha+\beta)} t_+^{\alpha+\beta-1} \\ &= Y_{\alpha+\beta}(t). \end{aligned} \quad (1.8)$$

The above result was obtained by change of variables and the property 2 from Proposition 1.1.2.

Remark 1.1.2. We suppose that the function f has some regularity (continuous, $L_{loc}^1(\mathbb{R}_+^*)$, causal function); The left-sided α -order Riemann–Liouville fractional integral

(1.3) can be rewritten as follows:

$${}_0I_t^\alpha f = D_{0,t}^{-\alpha} f := Y_\alpha \star f, \quad (1.9)$$

where $\alpha > 0$.

Remark 1.1.3. Thanks to the Remark 1.1.1 and Remark 1.1.2, yields:

$${}_0I_t^\alpha {}_0I_t^\beta = D_{0,t}^{-\alpha} D_{0,t}^{-\beta} = {}_0I_t^{\alpha+\beta} = D_{0,t}^{-\alpha-\beta}, \quad (1.10)$$

where $\alpha, \beta > 0$.

1.1.3 Fractional derivatives

Definition 1.1.8. The left-sided α -order Caputo fractional derivative of a function $f(t)$ is defined as

$${}^C D_{0,t}^\alpha f(t) = \begin{cases} {}^{\text{RL}} I_{0,t}^{n-\alpha} \left\{ \frac{d^n}{dt^n} f(t) \right\}, & \text{if } n-1 < \alpha < n \in \mathbb{Z}^+, \\ \frac{d^n}{dt^n} f(t), & \text{if } \alpha = n \in \mathbb{Z}^+. \end{cases} \quad (1.11)$$

Remark 1.1.4. According to the Definition 1.1.3, then the left-sided α -order Caputo fractional derivative of a function $f(t)$ can be expressed by the following explicit form:

$${}^C D_{0,t}^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-s)^{n-\alpha-1} \frac{d^n}{ds^n} f(s) ds, \quad \text{for } n-1 < \alpha < n, \quad (1.12)$$

where $n \in \mathbb{Z}^+$.

Definition 1.1.9. Let $f \in C^1([0, T])$, $T > 0$, $0 < \alpha(t) \leq 1$ and be continuous, the left-sided Caputo variable-order derivative is defined as follows:

$${}^C D_{0,t}^{\alpha(t)} f(t) = \begin{cases} {}_0I_t^{1-\alpha(t)} \left\{ \frac{d}{dt} f(t) \right\}, & \text{if } 0 < \alpha(t) < 1, \\ \frac{d}{dt} f(t), & \text{if } \alpha(t) = 1. \end{cases} \quad (1.13)$$

Definition 1.1.10. Let $f \in C^1([0, T])$, $T > 0$, and $\alpha \in (0, 1)$. The left-sided Caputo-Fabrizio fractional derivative of a function $f(t)$ is defined as

$${}^{\text{CF}}D_{0,t}^{\alpha} f(t) = \frac{M(\alpha)}{1-\alpha} \int_0^t \frac{d}{ds} f(s) \exp\left(-\frac{\alpha(t-s)}{1-\alpha}\right) ds. \quad (1.14)$$

Definition 1.1.11. Let $f \in C^1([0, T])$, $T > 0$, and $\alpha \in (0, 1)$. The left-sided Atangana-Baleanu fractional derivative in the Caputo sense of a function $x(t)$ is defined as

$${}^{\text{ABC}}D_{0,t}^{\alpha} f(t) = \frac{AB(\alpha)}{1-\alpha} \int_0^t \frac{d}{ds} f(s) E_{\alpha}\left(-\frac{\alpha(t-s)^{\alpha}}{1-\alpha}\right) ds, \quad (1.15)$$

where $E_{\alpha}(z)$ is the Mittag-Leffler kernel function of order α defined as

$$E_{\alpha}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad (1.16)$$

for $\alpha > 0$ and $z \in \mathbb{C}$.

Definition 1.1.12. The generalized function in the sense of Schwartz corresponding to $Y_{\alpha}(t)$ is denoted by $Y_{-\alpha}(t)$ and satisfies the convolution

$$Y_{+\alpha} \star Y_{-\alpha} = \delta,$$

where δ is the Dirac distribution. Note that δ here constitutes the neutral element of the convolution operation.

Definition 1.1.13. The generalized fractional derivative with order $\alpha > 0$ of a function or distribution f is defined as

$${}^{\text{G}}D_{0,t}^{\alpha} f = Y_{-\alpha} \star f.$$

The most important properties of the fractional integral/derivative that will be useful later are listed below.

Proposition 1.1.3. Let $\alpha, \beta > 0$, we have

1.
$${}^G D_{0,t}^\alpha {}^G D_{0,t}^\beta = {}^G D_{0,t}^{\alpha+\beta}. \quad (1.17)$$

2. For $f \in C^1([0, T])$ with $T > 0$, and $\alpha + \beta \leq 1$, then

$${}^C D_{0,t}^\alpha {}^C D_{0,t}^\beta f(t) = {}^C D_{0,t}^{\alpha+\beta} f(t). \quad (1.18)$$

3.

$$D_{0,t}^{-\alpha} {}^G D_{0,t}^\alpha f(t) = {}^G D_{0,t}^\alpha D_{0,t}^{-\alpha} f(t) = f(t). \quad (1.19)$$

4. For $n-1 < \alpha \leq n \in \mathbb{Z}^+$, and $f^{(n)} \in L^1_{loc}(\mathbb{R}_+^*)$, then

$${}^C D_{0,t}^\alpha f(t) = {}^G D_{0,t}^\alpha f(t) - \sum_{j=0}^{n-1} f^{(j)}(0) Y_{1+j-\alpha}(t). \quad (1.20)$$

Remark 1.1.5. For the property 2 in Proposition 1.1.3 the condition $\alpha + \beta \leq 1$ is important, we give a counterexample if this condition is not satisfied: Let $0 < \alpha, \beta < 1$ with $\alpha + \beta > 1$, and $f(t) = t$ with $t > 0$, then we have

$${}^C D_{0,t}^\beta {}^C D_{0,t}^\alpha f(t) = \frac{t^{1-\alpha-\beta}}{\Gamma(2-\alpha-\beta)} > 0, \quad \text{for } t > 0, \quad (1.21)$$

on the other hand, we have

$${}^C D_{0,t}^{\alpha+\beta} f(t) = \frac{1}{\Gamma(2-\alpha-\beta)} \int_0^t (t-s)^{1-\alpha-\beta} f^{(2)}(s) ds = 0. \quad (1.22)$$

1.2 Semigroup and their properties

Throughout this part, we denote by \mathcal{X} a real or complex Banach space provided with the norm $\|\cdot\|_{\mathcal{X}}$, $\mathcal{B}(\mathcal{X})$ the Banach algebra of bounded linear operators on \mathcal{X} , and \mathcal{I} the identity operator in $\mathcal{B}(\mathcal{X})$. We have relied on several references (see e.g. [7, 11, 12, 13, 23, 107]).

Definition 1.2.1. ([23]) A family $\{\mathcal{T}(t)\}_{t \in \mathbb{R}_+} \subset \mathcal{B}(\mathcal{X})$ is called a \mathcal{C}_0 -semigroup (or strongly semigroup) in \mathcal{X} , if it satisfies:

- i) $\mathcal{T}(t+s) = \mathcal{T}(s)\mathcal{T}(t)$ for all $t, s \in \mathbb{R}_+$,
- ii) $\mathcal{T}(0) = \mathcal{I}$,
- iii) $\lim_{t \rightarrow 0^+} \|\mathcal{T}(t)x - x\|_{\mathcal{X}} = 0$ for all $x \in \mathcal{X}$.

Definition 1.2.2. Let $d_i > 0$ for each $i = 1, \dots, N$. We define operators Λ_i , as follows

$$\Lambda_i \psi = d_i \Delta \psi \quad \text{for } \psi \in H_v^2(\Omega),$$

where

$$H_v^2(\Omega) := \left\{ \psi \in H^2(\Omega) \mid \frac{\partial \psi}{\partial \nu} = 0 \quad \text{on } \partial\Omega \right\} = D(\Lambda_i).$$

Definition 1.2.3. ([107]) Let $\alpha_i \in (0, 1)$, for $i \in \{1, \dots, N\}$, we define the operator families $\{\mathcal{S}_{\alpha_i}(t)\}_{t \geq 0}$, and $\{\mathcal{P}_{\alpha_i}(t)\}_{t \geq 0}$ by

$$\mathcal{S}_{\alpha_i}(t) = \int_0^\infty \Phi_{\alpha_i}(\sigma) \mathcal{T}_i(\sigma t^{\alpha_i}) d\sigma, \tag{1.23}$$

$$\mathcal{P}_{\alpha_i}(t) = \alpha_i \int_0^\infty \sigma \Phi_{\alpha_i}(\sigma) \mathcal{T}_i(\sigma t^{\alpha_i}) d\sigma,$$

where $\{\mathcal{T}_i(t)\}_{t \geq 0}$ is the semigroup generated by $-\Lambda_i$ and $\Phi_{\alpha_i}(\sigma)$ is the probability density function defined on \mathbb{R}_+^* by

$$\Phi_{\alpha_i}(\sigma) = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-\sigma)^n}{\Gamma(n)} \Gamma(n\alpha_i) \sin(n\pi\alpha_i).$$

Lemma 1.2.1. ([7]) When $t > 0$, $\alpha \in (0, 1)$ and $u \in C(\bar{\Omega})$, we have

1. $\|\mathcal{S}_\alpha(t)u(t)\|_\infty \leq \|u(t)\|_\infty$,

$$\| \| \quad 2. \|\mathcal{P}_\alpha(t)u(t)\|_\infty \leq \frac{1}{\Gamma(\alpha)} \|u(t)\|_\infty.$$

1.3 Derivation of mathematical models

In this part, we present how to model phenomena that depend on kinetics and diffusion (especially, chemical reactions) on fixed as well as moving (time-dependent, evolving) spacial domains, by applying a set of physical laws.

1.3.1 Reaction-diffusion equations on static spacial domains

Since in this thesis we deal with mathematical reaction-diffusion systems, we outline the derivation of the reaction-diffusion equations on static spatial domain. Let

$$u(x, t) = (u_1(x, t), u_2(x, t), \dots, u_m(x, t))^T,$$

be a vector of (chemical concentrations, ions, population densities, etc.) of species \mathcal{U}_i ($i = 1, \dots, m$) at a position $x = (x_1, \dots, x_N)^T \in \Omega \subset \mathbb{R}^N$ (Ω is bounded, simply connected and smooth) and at a time $t \in \mathbb{R}_+$. We denote by J_i ($i = 1, \dots, m$) by the flux of species \mathcal{U}_i and f_i by its net production rates. Due to the law of conservation of mass¹, we get

$$\frac{d}{dt} \int_\Omega u_i = - \int_{\partial\Omega} J_i \cdot \mathbf{v} + \int_\Omega f_i, \quad (i = 1, \dots, m), \quad (1.24)$$

where \mathbf{v} is the unit outward normal to $\partial\Omega$. Then, (1.24) reads (chemical viewpoint), the rate of change of a chemical concentration u_i in an arbitrary domain Ω is equal to the sum of the net flux of the chemical concentration through the boundary of the domain Ω (i.e. $\partial\Omega$) and the net production f_i of the chemical concentration within the domain Ω . According to the divergence theorem², (1.24) becomes:

$$\frac{d}{dt} \int_\Omega u_i = - \int_\Omega \nabla \cdot J_i + \int_\Omega f_i, \quad (i = 1, \dots, m). \quad (1.25)$$

¹**The law of conservation of mass** states that (in physics and chemistry) for any system closed to all transfers of matter and energy, the mass is neither created nor destroyed.

²**The divergence theorem:** If \mathcal{F} is a continuously differentiable vector field defined on a neighborhood of Ω , then:

$$\int_{\partial\Omega} \mathcal{F} \cdot \mathbf{v} = \int_\Omega \nabla \cdot \mathcal{F}$$

The differential operator and integral can be interchanged because the spacial domain Ω is independant of temporal variable t , then (1.25) leads to the following:

$$\int_{\Omega} \left(\frac{\partial u_i}{\partial t} + \nabla \cdot J_i - f_i \right) = 0, \quad (i = 1, \dots, m). \quad (1.26)$$

Since the integration in (1.26) holds on arbitrary (bounded, simply connected) domain Ω , and the integrand is continuous, thus

$$\frac{\partial u_i}{\partial t} = -\nabla \cdot J_i + f_i, \quad (i = 1, \dots, m). \quad (1.27)$$

The fluxes J_i and the functions f_i must now be modeled by adequate and constitutive laws. When the transport of mass is only related to diffusion, in 1855 a simple model was introduced by A. Fick [37]. According to Fick's law the flux J_i is proportional to the gradient of concentration u_i and given by:

$$J_i = -d_i \nabla u_i(x, t), \quad (i = 1, \dots, m), \quad (1.28)$$

where $d_i > 0$. Based on (1.27) and (1.28), we get

$$\frac{\partial u_i}{\partial t} = d_i \Delta u_i + f_i, \quad (i = 1, \dots, m), \quad (1.29)$$

for each $i = 1, \dots, m$, the functions $f_i := f_i(x, t, u(x, t))$ (the dependence on $u(x, t)$ being often nonlinear) can be obtained by using the law of mass action³ or by observations and experimental methods.

In order to the well-defined of differential problem we need to specify initial conditions and boundary conditions. The most common boundary conditions are homogeneous Neumann boundary conditions (zero-flux), which gives by the following mathematical expression:

$$\frac{\partial u_i}{\partial \nu} := \nu \cdot \nabla u_i = 0, \quad (i = 1, \dots, m). \quad (1.30)$$

Hence, a system expresses reaction-diffusion of m -species ($2 \leq m \in \mathbb{N}$) on static domain Ω , as follows:

$$\left\{ \begin{array}{ll} \frac{\partial u_i}{\partial t} - d_i \Delta u_i = f_i(x, t, u) & \text{in } \Omega \times \mathbb{R}_+^*, \quad i = 1, \dots, m, \\ \frac{\partial u_i}{\partial \nu} = 0 & \text{on } \partial\Omega \times \mathbb{R}_+^*, \quad i = 1, \dots, m, \\ u_i(x, 0) = u_{0i}(y) & \text{on } \bar{\Omega}, \quad i = 1, \dots, m, \end{array} \right. \quad (1.31)$$

³The law of mass action states that the rate of the chemical reaction is directly proportional to the product of the activities or concentrations of the reactants.

1.3.2 Reaction-diffusion equations on evolving spacial domains

Throughout this subsection, We have relied on several references (see e.g. [15, 64]). Consider a simply connected, bounded, time-dependent domain $\Omega_t \subset \mathbb{R}^N$ ($N \geq 1$) with a moving boundary $\partial\Omega_t$ that is smooth ($t \in [0, \tilde{t}]$, $\tilde{t} > 0$). The domain Ω_t can be mapped into a static reference domain Ω_0 by using a C^k -diffeomorphism ($k \geq 2$) $\rho_t : \Omega_0 \rightarrow \Omega_t$, i.e., for each $x := x(t) \in \Omega_t$ there exists $y \in \Omega_0$ such that (see Figure 1.1):

$$x = \rho_t(y). \quad (1.32)$$

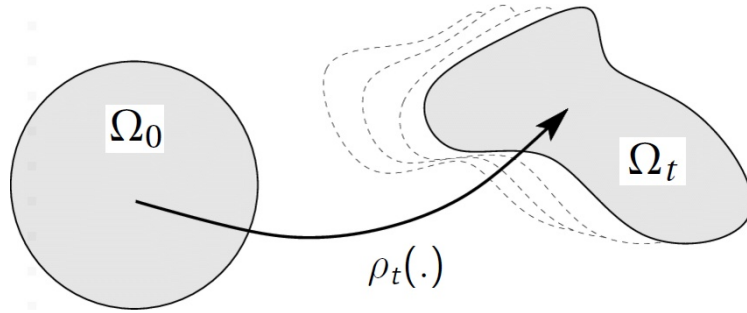


Figure 1.1: Diffeomorphism ρ_t between evolving domain Ω_t and static domain Ω_0 .

Moreover, the diffeomorphism ρ_t is assumed to be a C^2 function with respect to t . The change in the volume of domain Ω_t generates a flow of velocity denoted by

$$\vartheta(x, t) = \vartheta(\rho_t(y), t) := \frac{\partial \rho_t(y)}{\partial t}, \quad x \in \Omega_t, \quad y \in \Omega_0. \quad (1.33)$$

In the following, we need the following result:

$$\frac{\partial \Xi(y, t)}{\partial t} = (\nabla \cdot \vartheta(\rho_t(y), t)) \Xi(y, t), \quad (1.34)$$

where $\Xi(y, t)$ denotes the determinant of the Jacobian $\mathcal{J}(y, t) = D\rho_t(y)$ of the diffeomorphism ρ_t (i.e. $\Xi(y, t) = \det(\mathcal{J}(y, t))$).

After this configuration, we are now ready to begin the process of deriving the equations of reaction-diffusion on time-dependant domain. As in the previous section, let

$$u(x, t) := (u_1(x, t), u_2(x, t), \dots, u_m(x, t))^T,$$

be a vector of (chemical concentrations, ions, population densities, etc.) of species \mathcal{U}_i ($i = 1, \dots, m$) at a position $x := x(t) = (x_1(t), \dots, x_N(t))^T \in \Omega_t \subset \mathbb{R}^N$ and at a time $t \in \mathbb{R}_+$. We denote by J_i ($i = 1, \dots, m$) by the flux of species \mathcal{U}_i and f_i by its net production

rates. According to the law of conservation of mass and divergence theorem with time-dependant domain, we get

$$\frac{d}{dt} \int_{\Omega_t} u_i = - \int_{\Omega_t} \nabla \cdot J_i + \int_{\Omega_t} f_i, \quad (i = 1, \dots, m). \quad (1.35)$$

Unlike the static domain, in this case the differential operator cannot be pass through integration on a time-dependant domain. We deal with the left side of (1.35) separately, for each $i = 1, \dots, m$, we have

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_t} u_i(x, t) &= \frac{d}{dt} \int_{\Omega_0} u_i(\rho_t(y), t) \Xi(y, t) \\ &= \int_{\Omega_0} \frac{d}{dt} (u_i(\rho_t(y), t) \Xi(y, t)) \\ &= \int_{\Omega_0} \Xi(y, t) \frac{d u_i(\rho_t(y), t)}{dt} + u_i(y, t) \frac{\partial \Xi(y, t)}{\partial t}, \end{aligned} \quad (1.36)$$

thanks to (1.33), (1.34) and differentiation rules, for each $i = 1, \dots, m$, we obtain

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_t} u_i(x, t) &= \int_{\Omega_0} \left[\frac{d u_i(\rho_t(y), t)}{dt} + u_i(\nabla \cdot \vartheta) \right] \Xi \\ &= \int_{\Omega_0} \left[\frac{d u_i(\rho_t(y), t)}{dt} + u_i(\nabla \cdot \vartheta) \right] \Xi \\ &= \int_{\Omega_0} \left[\frac{\partial u_i}{\partial t} + \frac{\partial \rho_t(y)}{\partial t} \cdot \nabla u_i + u_i(\nabla \cdot \vartheta) \right] \Xi \\ &= \int_{\Omega_t} \frac{\partial u_i}{\partial t} + \vartheta \cdot \nabla u_i + u_i(\nabla \cdot \vartheta) \\ &= \int_{\Omega_t} \frac{\partial u_i}{\partial t} + \nabla \cdot (u_i \vartheta). \end{aligned} \quad (1.37)$$

The equality (1.37) is known by Reynolds transport theorem. Now, by combining (1.35) and (1.37), we get

$$\int_{\Omega_t} \left(\frac{\partial u_i}{\partial t} + \nabla \cdot (u_i \vartheta) + \int_{\Omega_t} \nabla \cdot J_i - f_i \right) = 0, \quad (i = 1, \dots, m). \quad (1.38)$$

By completing as in the previous sub-section (reaction-diffusion system on static domain), we reach to the final equations of reaction-diffusion (taking into account the homogeneous Neumann boundary conditions) on time-varying domain:

$$\left\{ \begin{array}{ll} \frac{\partial u_i}{\partial t} + \nabla \cdot (u_i \vartheta) - d_i \Delta u_i = f_i(x, t, u) & \text{in } \Omega_t \times \mathbb{R}_+^*, i = 1, \dots, m, \\ \frac{\partial u_i}{\partial \nu} = 0 & \text{on } \partial \Omega_t \times \mathbb{R}_+^*, i = 1, \dots, m, \\ u_i(x, 0) = u_{0i}(y) & \text{on } \overline{\Omega}_0, i = 1, \dots, m. \end{array} \right. \quad (1.39)$$

1.4 Some basic results about reaction-diffusion equations

In this section, we will present the most important findings about reaction-diffusion systems (1.31), represented in local existence & uniqueness of solution, comparison principle, and positivity of solution.

1.4.1 Local existence of solutions

The following basic assumptions on system (1.31) are assumed to hold:

(BA1) $f = (f_i)_{i=1}^m : \overline{\Omega} \times \mathbb{R}_+ \times \mathbb{R}_+^m \longrightarrow \mathbb{R}^m$ is locally Lipschitz in each variable.

(BA2) $u_0 = (u_{0i})_{i=1}^m \in L^\infty(\Omega; \mathbb{R}^m)$.

Before declaring the main result in this sub-section we will need this definition (see [82]):

Definition 1.4.1. A function $u := (u_1, \dots, u_m)$ is a classical solution to (1.31) on $(0, T)$ if, for $i = 1, \dots, m$, we have:

$$u_i \in C^{2,1}(\overline{\Omega} \times (0, T)) \cap C([0, T]; L^\infty(\Omega)),$$

and u satisfies (1.31).

The local existence of solution of system (1.31) follows from classical results, as follows:

Theorem 1.4.1. ([48, 92]) Suppose that (BA1)-(BA2) hold. Then the system (1.31) admits a unique, classical solution on $\Omega \times [0, T_{max})$ where $0 < T_{max} \leq \infty$. Moreover,

$$\text{if } T_{max} < +\infty, \text{ then } \lim_{t \rightarrow T_{max}} \sum_{i=1}^m \|u_i(\cdot, t)\|_{L^\infty(\Omega)} = +\infty. \quad (1.40)$$

Remark 1.4.1. Thanks to (1.40), to prove global existence (i.e. $T_{max} = +\infty$) of classical solution for system (1.31), it is sufficient to get that:

$$\forall t \in [0, T_{max}), \quad \sum_{i=1}^m \|u_i(\cdot, t)\|_{L^\infty(\Omega)} \leq \mathcal{G}(t), \quad (1.41)$$

where $\mathcal{G} \in C(\mathbb{R}_+, \mathbb{R}_+)$, and is nondecreasing function.

1.4.2 Comparaison principle and positivity of solutions

First, we will present an important theorem that helps in obtaining initial estimates for solutions of reaction-diffusion systems, known as the comparaison principle:

Theorem 1.4.2. ([92]) Let $T > 0$, if the functions

$$u := (u_1, \dots, u_m), v := (v_1, \dots, v_m) \in \left[C^{2,1}(\overline{\Omega} \times (0, T)) \right]^m, \quad (1.42)$$

satisfy

$$\frac{\partial u_i}{\partial t} - d_i \Delta u_i - f_i(x, t, u) \leq \frac{\partial v_i}{\partial t} - d_i \Delta v_i - f_i(x, t, v), \quad \text{in } \Omega \times (0, T), i = 1, \dots, m, \quad (1.43)$$

$$u_{0i}(x) \leq v_{0i}(x), \quad \text{in } \Omega, i = 1, \dots, m, \quad (1.44)$$

$$\frac{\partial u_i}{\partial \nu} = \frac{\partial v_i}{\partial \nu} = 0, \quad \text{on } \partial\Omega \times (0, T), i = 1, \dots, m. \quad (1.45)$$

Then

$$u_i(x, t) \leq v_i(x, t), \quad \text{in } \overline{\Omega} \times (0, T], i = 1, \dots, m. \quad (1.46)$$

Since the properties of chemical concentration, density of population, number of individuals, ... ect, are positive quantities (either in the initial stage or after a period of time), then we need to elicit this property in system (1.31). Before showing the positivity of solution of (1.31), we need the following precondition:

Definition 1.4.2. (Quasi-positive function) The nonlinearity $f = (f_i)_{i=1}^m$ (in system (1.31)) is called quasi-positive if satisfies:

$$\forall u = (u_1, \dots, u_m) \in \mathbb{R}_+^m, \quad \forall i = 1, \dots, m, \quad f_i(u_1, \dots, u_{i-1}, 0, u_{i+1}, \dots, u_m) \geq 0. \quad (1.47)$$

According to the comparison principle and the precondition stated above, we get the following result about positivity of solution for system (1.31).

Corollary 1.4.1. ([85]) Suppose that (BA1)-(BA2) hold, moreover, the nonlinearity $f = (f_i)_{i=1}^m$ is quasi-positive. Then the system (1.31) admits a unique, classical solution on $\Omega \times [0, T_{max})$ where, for $i = 1, \dots, m$

$$\forall x \in \Omega, \quad u_{0i}(x) \geq 0 \implies \forall (x, t) \in \Omega \times [0, T_{max}), \quad u_i(x, t) \geq 0. \quad (1.48)$$

1.4.3 Global existence of solutions for reaction-diffusion equations

Consider the initial-boundary value problem (semilinear parabolic equation):

$$\begin{cases} \frac{\partial u}{\partial t} - d\Delta u = f(x, t, u) & \text{in } \Omega \times \mathbb{R}_+^*, \\ \frac{\partial u}{\partial \nu}(x, t) = 0 & \text{on } \partial\Omega \times \mathbb{R}_+^*, \\ u(x, 0) = u_0(x) & \text{in } \bar{\Omega}. \end{cases} \quad (1.49)$$

Where $\Omega \subset \mathbb{R}^N$ (Ω is bounded, simply connected and smooth), and $d > 0$. Furthermore, we assume:

(LEA1) $f : \Omega \times \mathbb{R}_+^* \times \mathbb{R} \rightarrow \mathbb{R}$ is locally Lipschitzian function of all its arguments.

(LEA2) $u_0 \in C(\bar{\Omega})$.

Under the above assumptions (LEA1)-(LEA2), The problem (1.49) admits a unique classical solution on $\Omega \times [0, T_{max})$ where $0 < T_{max} \leq \infty$. Moreover, we have the same characterization of T_{max} (see (1.40) with $m = 1$, and $u \equiv u_1$).

In light of the Remark 1.4.1, we conclude that the assumptions (LEA1)-(LEA2) are not enough to guarantee the global existence of solution for (1.49). Indeed, this is what the following example shows:

Example 1.4.1. Let the initial-boundary value (special case of problem (1.49)):

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = u^2 & \text{in } \Omega \times \mathbb{R}_+^*, \\ \frac{\partial u}{\partial \nu}(x, t) = 0 & \text{on } \partial\Omega \times \mathbb{R}_+^*, \\ u(x, 0) = u_0(x) & \text{in } \bar{\Omega}. \end{cases} \quad (1.50)$$

Where $u_0 \in C(\bar{\Omega}; \mathbb{R}_+)$, then the assumptions (LEA1)-(LEA2) hold. Furthermore, we assume that

$$\int_{\Omega} u_0(x) dx > 0. \quad (1.51)$$

Thus, the problem (1.50) has a unique nonnegative classical solution on $\Omega \times [0, T_{max})$.

On the other hand, integrating the first equation of (1.50) with respect to the spatial variable, we obtain

$$\frac{d}{dt} \int_{\Omega} u(x, t) dx = \int_{\Omega} u^2(x, t) dx, \quad (1.52)$$

by means the Holder's inequality, we get

$$\frac{d}{dt} \int_{\Omega} u(x, t) dx = \int_{\Omega} u^2(x, t) dx \geq \frac{1}{|\Omega|} \left(\int_{\Omega} u(x, t) dx \right)^2. \quad (1.53)$$

The solution of the differential inequality (1.53) has the following form:

$$\int_{\Omega} u(x, t) dx \geq \frac{\mathcal{C} |\Omega|}{|\Omega| - \mathcal{C} t}, \quad (1.54)$$

where $\mathcal{C} := \int_{\Omega} u_0(x) dx$. Hence

$$\lim_{t \rightarrow \frac{|\Omega|}{\mathcal{C}}} \int_{\Omega} u(x, t) dx = +\infty. \quad (1.55)$$

Thus, the solution of (1.50) blow-up (does not global) in the finite time $T_{max} := \frac{|\Omega|}{\mathcal{C}}$.

Based on the foregoing, it is clear that conditions must be posed on the inputs of the problem (1.49) in order to ensure the global existence of solution. This is what the following theorem addresses:

Theorem 1.4.3. ([44, 46, 56, 92]) Suppose that (LEA1)-(LEA2) hold. Moreover, we assume for $p > \frac{N}{2}$,

$$f(x, \cdot, u) \in L^\infty((0, T_{\max}); L^p(\Omega)), \quad \forall (x, u) \in \Omega \times \mathbb{R}. \quad (1.56)$$

Then, the unique solution of (1.49) exists globally (i.e. $T_{\max} = +\infty$).

Remark 1.4.2. Practically, to deal with the system (1.31) we need to deal separately with m -initial-boundary value problems as in (1.49).

Remark 1.4.3. To get the condition (1.56), priori estimates on (1.31) (taking into account the Remark 1.4.2) can be used, or a suitable Lyapunov function⁴, ... etc.

1.5 General Activator-inhibitor model

Consider a 2-species in reaction-diffusion system (1.31) (i.e. $m = 2$):

$$\frac{\partial u}{\partial t} = d_u \Delta u + f_1(u, v), \quad \frac{\partial v}{\partial t} = d_v \Delta v + f_2(u, v). \quad (1.57)$$

Assume there exists a constant steady-state $E_{eq} := (u_{eq}, v_{eq})$,

$$f_1(u_{eq}, v_{eq}) = f_2(u_{eq}, v_{eq}) = 0.$$

The Jacobian of the system (1.57) at E_{eq} is defined by:

$$J|_{E_{eq}} = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} := \begin{pmatrix} \left. \frac{\partial f_1}{\partial u} \right|_{E_{eq}} & \left. \frac{\partial f_1}{\partial v} \right|_{E_{eq}} \\ \left. \frac{\partial f_2}{\partial u} \right|_{E_{eq}} & \left. \frac{\partial f_2}{\partial v} \right|_{E_{eq}} \end{pmatrix}.$$

We say that the reaction diffusion system is the inhibitory activator system if the coefficients of its Jacobian matrix have the following relationships:

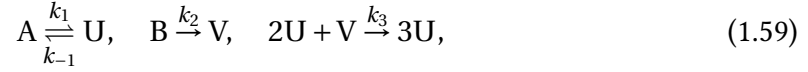
$$J_{11}J_{22} < 0, \quad J_{12}J_{21} < 0. \quad (1.58)$$

⁴Lyapunov functional associated with system (1.31): It is each function $\mathcal{L} : \mathbb{R}_+ \rightarrow \mathbb{R}_+$, satisfies

$$\frac{d}{dt} \mathcal{L}(u(\cdot, t)) \leq 0, \quad \forall (t, u) \in \mathbb{R}_+^* \times \mathbb{R}_+^m.$$

The corresponding species that achieves $J_{ii} > 0$, ($J_{ii} < 0$) for $i = 1, 2$, is called activator (inhibitor), respectively.

Example 1.5.1. The Schnakenberg model is a simple system of reaction-diffusion equations occurring in chemical kinetics and biological processes. It was first proposed by Schnakenberg in 1979 (cf. [97]). The Schnakenberg chemical reaction can be represented by the following mechanism:



where A, B, U and V are chemical reactants and products. The steps in (1.59) yield the nondimensionalized Schnakenberg reaction-diffusion system:

$$\begin{cases} \frac{\partial u}{\partial t} - d_1 \Delta u = a - u + u^2 v =: f_1(u, v), & x \in \Omega, t > 0, \\ \frac{\partial v}{\partial t} - d_2 \Delta v = b - u^2 v =: f_2(u, v), & x \in \Omega, t > 0. \end{cases} \quad (1.60)$$

Subject to the homogeneous Neumann boundary conditions and initial data. In this system, the reactions occur in a domain $\Omega \subset \mathbb{R}^N$ (with $N \in \mathbb{N}^*$), $u := u(x, t)$ and $v := v(x, t)$ are the chemical concentrations of an activator and an inhibitor, respectively, and d_1, d_2, a, b are positive numbers, such that $b > a$. In this case, it is clear that the condition (1.58) is satisfied.

CHAPTER

2

TIME-FRACTIONAL REACTION-DIFFUSION SYSTEMS

“My work always tried to unite the truth with the beautiful, but when I had to choose one or the other, I usually chose the beautiful.”

Hermann Weyl

This chapter concerns with a qualitative analysis of reaction-diffusion systems involving fractional derivative in Caputo sense respect to time variable. The results appearing in this context have been published through [\[31\]](#).

Understanding the dynamics and nature of solutions for such systems has been the subject of study by mathematicians and scientists for many decades. One of major interests of researchers is the asymptotic stability of the solutions. Until a few decades ago, interest in reaction-diffusion systems was limited to integer order derivatives both in time and space. Although the inception of fractional calculus is centuries old, it was not until recently that its practical meaning was noticed [\[25, 66, 94, 98\]](#). It has been noticed that fractional differential equations can represent a variety of problems more accurately and efficiently, especially nonlocal problems such as anomalous diffusion [\[19\]](#) and the modeling of materials with a memory [\[47\]](#).

Since the fractional derivative in Caputo sense is a generalization of the classical derivative, so the models that include the fractional derivative show a richness in their dynamics, and this allows us to approach more than accurate modeling of phenomena. Precisely, this chapter establishes conditions for the asymptotic stability of time-fractional reaction-diffusion systems. The stability of linear systems is investigated by means of the eigenfunction expansion of the Laplacian operator. Theoretical bounds are placed on the arguments of the infinity of eigenvalues belonging to the instant Jacobian matrix. Nonlinear systems are linearized by means of their Taylor series expansion. Numerical solutions of two real-istic examples are presented to illustrate the theoretical findings.

The considered system

Let Ω be a bounded domain in $\mathbb{R}^{N'}$, with a smooth boundary $\partial\Omega$. In this section we present the existence of solution for the time-fractional reaction diffusion system, of the form:

$${}^C D_{0,t}^{\hat{\alpha}} u(t, x) = D\Delta u(t, x) + Au(t, x), \quad t > 0, x \in \Omega, \quad (2.1)$$

with initial conditions

$$u(0, x) = u_0(x), \quad x \in \Omega, \quad (2.2)$$

and homogeneous Neumann boundary conditions, i.e.

$$(v \cdot \nabla) u(t, x) = 0, \quad t > 0, x \in \partial\Omega, \quad (2.3)$$

where, $u(x, t) = (u_1(t, x), \dots, u_N(t, x))^T$ and $N, N' \in \mathbb{N}$, $A = (a_{i,j})_{1 \leq i, j \leq N}$ is a real constant matrix, $D = \text{diag}(d_1, \dots, d_N)$ with $d_i > 0$ for $i = 1, \dots, N$ and ${}^C D_{0,t}^{\hat{\alpha}} = ({}^C D_{0,t}^{\alpha_1}, \dots, {}^C D_{0,t}^{\alpha_N})^T$, v is the unit outward normal to $\partial\Omega$.

In this chapter, we are interested in establishing sufficient theoretical conditions for the asymptotic stability of time–fractional reaction–diffusion systems (2.1)-(2.3) and also for the nonlinear reaction function.

The background related to the subject can be divided into two major parts, the stability of fractional ODEs and the stability of integer–order reaction–diffusion systems. The stability of fractional differential equations has been studied by many including [69], where Matignon derived an upper bound on the arguments of the Jacobian eigenvalues below which the system is guaranteed to be asymptotically stable. This work was later extended in [26] for systems with multiple time delays. In their study, Deng *et al.* also treated the incommensurate case, where the fractional orders of the system equations are non–identical. Further results on the stability of incommensurate fractional ODE systems were reported in [84] and [61]. In [58], Lenka *et al.* extended the results to systems with fractional derivatives of an order in the range 0 to 2. Other relevant studies include [76], where Odibat examined a range of issues related to this type of systems

including the existence and uniqueness of solutions as well as their stability. In addition, the solutions of such systems in the commensurate and incommensurate cases by means of Mittag-Leffler functions was examine in [35].

The stability of nonlinear reaction diffusion systems relies mainly on linearization about the system's constant steady-state, which was first applied in [79]. The mathematical justification for this technique came later on in [18, 17]. In [108], Wang and Li derived a set of stability conditions, which they called the minor condition for the stability of constant steady-state solutions to reaction-diffusion systems with Neumann boundary conditions. More recent works include [75, 41]. For more on the stability of specific commensurate time-fractional reaction-diffusion systems, the reader may wish to refer to [22, 114, 115] and references therein.

2.1 Existence of solutions

In this section, we address the existence of solutions for the system (2.1)-(2.3). We have inspired by the literature [91, 113]. The following definitions will be useful later on.

Definition 2.1.1. Let $T > 0$ and $(u_{01}, \dots, u_{0N}) \in [C(\bar{\Omega})]^N$, a vector function

$$(u_1, \dots, u_N) \in C\left([0, T]; [C(\bar{\Omega})]^N\right),$$

is called a mild solution of (2.1)-(2.3), if for each $i \in \{1, \dots, N\}$, u_i satisfy

$$u_i(t) = \mathcal{S}_{\alpha_i}(t)u_{0i} + \sum_{j=1}^N a_{ij} \int_0^t (t-s)^{\alpha_i-1} \mathcal{P}_{\alpha_i}(t-s)u_j(s),$$

where $u_i(t) = u_i(t, \cdot)$, $\mathcal{S}_{\alpha_i}(t)$ and \mathcal{P}_{α_i} are mentioned in definition 1.2.3.

Definition 2.1.2. A vector function $u \in C\left([0, T]; [C(\bar{\Omega})]^N\right)$ is called a classical solution of the problem (2.1)-(2.3) if u is continuously differentiable of order $\hat{\alpha} = (\alpha_1, \dots, \alpha_N)$ on $(0, T]$, for all $t \in [0, T]$, $u(t) \in D(\Lambda_1) \times \dots \times D(\Lambda_N)$ and satisfies (2.1)-(2.3).

The following proposition presents the existence of mild solution of the initial-boundary problem (2.1)-(2.3), which is our preliminary result.

Proposition 2.1.1. Let $(u_{01}, \dots, u_{0N}) \in [C(\bar{\Omega})]^N$, then the problem (2.1)-(2.3) for $\alpha_i \in (0, 1)$, $i \in \{1, \dots, N\}$ has a unique mild solution.

Proof. Consider the Banach space $\mathfrak{X} := C([0, T]; [C(\bar{\Omega})]^N)$ with the norm

$$\|u\|_{\mathfrak{X}} = \|(u_1, \dots, u_N)\|_{\mathfrak{X}} := \sup_{t \in [0, T]} e^{-kt} \|u(t)\|_{N, \infty},$$

where $k \in \mathbb{N}$ which will be fixed later and $\|u(t)\|_{N, \infty} := \sum_{i=1}^N \|u_i(t)\|_{\infty}$. We define the operator

$\Upsilon = (\Upsilon_1, \dots, \Upsilon_N)$ on \mathfrak{X} , where

$$(\Upsilon_i u)(t) = \mathcal{S}_{\alpha_i}(t) u_{0i} + \sum_{j=1}^N a_{ij} \int_0^t (t-s)^{\alpha_i-1} \mathcal{P}_{\alpha_i}(t-s) u_j(s) ds.$$

By the properties of $\mathcal{S}_{\alpha_i}(t)$ and $\mathcal{P}_{\alpha_i}(t)$ (see e.g. [39, 107]) we can get that $\Upsilon u \in \mathfrak{X}$ when $u \in \mathfrak{X}$. So Υ maps \mathfrak{X} into itself, then the mild solution of the problem (2.1)-(2.3) is the fixed point of Υ .

Assume that $u, v \in \mathfrak{X}$, for each $t \in [0, T]$ and each $i \in \{1, \dots, N\}$. Using Lemma 1, we have

$$\begin{aligned} \|(\Upsilon_i u)(t) - (\Upsilon_i v)(t)\|_{\infty} &\leq \frac{\mathcal{C}_i}{\Gamma(\alpha_i)} \int_0^t (t-s)^{\alpha_i-1} \|u(s) - v(s)\|_{N, \infty} ds \\ &= \frac{\mathcal{C}_i}{\Gamma(\alpha_i)} \int_0^t (t-s)^{\alpha_i-1} e^{-ks} \|u(s) - v(s)\|_{N, \infty} e^{ks} ds \\ &\leq \frac{\mathcal{C}_i}{\Gamma(\alpha_i)} \|u - v\|_{\mathfrak{X}} \int_0^t (t-s)^{\alpha_i-1} e^{ks} ds \\ &\leq \frac{\mathcal{C}_i}{k^{\alpha_i}} e^{kt} \|u - v\|_{\mathfrak{X}}, \end{aligned}$$

where $\mathcal{C}_i = \|(a_{i1}, \dots, a_{iN})\|_{\mathbb{R}^N}$, thus

$$\|\Upsilon u - \Upsilon v\|_{\mathfrak{X}} \leq \sum_{i=1}^N \frac{\mathcal{C}_i}{k^{\alpha_i}} \|u - v\|_{\mathfrak{X}}.$$

We can choose $k \in \mathbb{N}$ large enough such that

$$\sum_{i=1}^N \frac{\mathcal{C}_i}{k^{\alpha_i}} < 1.$$

Hence, Υ is a strict contraction on \mathfrak{X} . Thus, by the Banach's fixed point theorem, Υ has a fixed point $u \in \mathfrak{X}$.

Now, we prove the uniqueness. Let $u, v \in \mathfrak{X}$ be two mild solutions of (2.1)–(2.3) for $T > 0$, then we have

$$\begin{aligned} \|u_i(t) - v_i(t)\|_\infty &= \|(Y_i u)(t) - (Y_i v)(t)\|_\infty \\ &\leq \frac{\mathcal{C}_i}{\Gamma(\alpha_i)} \int_0^t (t-s)^{\alpha_i-1} \|u(s) - v(s)\|_{N,\infty} ds. \end{aligned}$$

Hence

$$\|u(t) - v(t)\|_{N,\infty} \leq \mathcal{C} \int_0^t \sum_{i=1}^N (t-s)^{\alpha_i-1} \|u(s) - v(s)\|_{N,\infty} ds,$$

where $\mathcal{C} = \max\left\{\frac{\mathcal{C}_1}{\Gamma(\alpha_1)}, \dots, \frac{\mathcal{C}_N}{\Gamma(\alpha_N)}\right\}$. Thus, by Gronwall's inequality, we get that $u = v$. ■

Remark 2.1.1. We can extend the result in the Proposition 1 for $\alpha_i \in (0, 1]$, $i \in \{1, \dots, N\}$, so that for each $i \in \{1, \dots, N\}$ we put

$$(Y_i u)(t) = \begin{cases} \mathcal{S}_{\alpha_i}(t)u_{0i} + \sum_{j=1}^N a_{ij} \int_0^t (t-s)^{\alpha_i-1} \mathcal{P}_{\alpha_i}(t-s)u_j(s)ds & \text{if } \alpha_i \in (0, 1), \\ \mathcal{T}_i(t)u_{0i} + \sum_{j=1}^N a_{ij} \int_0^t \mathcal{T}_i(t-s)u_j(s)ds & \text{if } \alpha_i = 1. \end{cases}$$

For the classical derivative (see [106]). The following result is concerning the regularity of the mild solution.

Corollary 2.1.1. For each $u_0 \in D(\Lambda_1) \times \dots \times D(\Lambda_N)$, and $u \in C\left([0, T]; \left[C(\overline{\Omega})\right]^N\right)$ is a mild solution of the problem (2.1)–(2.3) for $\alpha_i \in (0, 1]$, $i \in \{1, \dots, N\}$, then u is a classical solution of the problem (2.1)–(2.3).

Proof. By the same argument as in [106, 107].

2.2 Asymptotic stability conditions for autonomous time–fractional reaction–diffusion systems

Throughout this section, we will present our most important results about asymptotic stability for autonomous time–fractional reaction–diffusion systems.

2.2.1 Stability criteria for linear fractional reaction–diffusion systems

In the following, we discuss the asymptotic stability criteria for system (2.1)–(2.3) in the commensurate and incommensurate scenarios.

2.2.1.1 Commensurate scenario

Let us start by assessing the stability of the solutions to the generalized linear time–fractional reaction diffusion system (2.1)–(2.3) subject to the fractional orders being identical, i.e. $\alpha_1 = \dots = \alpha_N = \alpha \in (0, 1]$. First, we must define some important notation to be used in the proofs. We denote by $\left\{ \lambda_i, \{w_{ij}\}_{j=1}^{m_i} \right\}_{i=0}^{\infty}$ an eigenpair of the elliptic operator $(-\Delta)$ on Ω subject to Neumann boundary conditions where $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$. The algebraic multiplicity of the eigenvalue λ_i is $m_i \in \mathbb{N}$. We also denote the eigenspace corresponding to λ_i as Ξ_{ij} and define

$$\Xi_i = \bigoplus_{j=1}^{m_i} \Xi_{ij},$$

and the sets

$$\Xi = \left\{ (u_1, \dots, u_N)^\top \in \left[C^2(\Omega) \cap C(\bar{\Omega}) \right]^N \mid (v \cdot \nabla) u_k = 0, \text{ in } \partial\Omega, k = 1, \dots, N \right\}, \quad (2.4)$$

and

$$\Xi_{ij} = \{c w_{ij} \mid c \in \mathbb{R}^N\}.$$

Also, let us set define the operator

$$L = D\Delta + A. \quad (2.5)$$

Finally, note that Ξ can be decomposed in the form

$$\Xi = \bigoplus_{i=0}^{\infty} \Xi_i. \quad (2.6)$$

Theorem 2.2.1. Subject to $\alpha_1 = \dots = \alpha_N = \alpha \in (0, 1]$, if for all $i \in \mathbb{N}_0$ both the roots of the characteristic equation

$$\det(A - \lambda_i D - \mu I) = 0, \quad (2.7)$$

satisfy the criterion

$$|\arg(\mu)| > \frac{\alpha\pi}{2},$$

then the zero solution of system (2.1)–(2.3) is asymptotically stable. On the contrary, if at least one root of at least one equation of (2.7) satisfies $|\arg(\mu)| < \frac{\alpha\pi}{2}$, then the zero solution of (2.1)–(2.3) becomes asymptotically unstable.

Proof. The characteristic equation can be given by

$$L(\Phi_1, \dots, \Phi_N)^\top = \mu(\Phi_1, \dots, \Phi_N)^\top. \quad (2.8)$$

Since

$$(\Phi_1, \dots, \Phi_N)^\top = \sum_{i=0}^{\infty} \sum_{j=1}^{m_i} (a_{1ij}, \dots, a_{Nij})^\top w_{ij}, \quad (2.9)$$

we obtain

$$\sum_{i=0}^{\infty} \sum_{j=1}^{m_i} (A - \lambda_i D - \mu I) (a_{1ij}, \dots, a_{Nij})^\top w_{ij} = 0. \quad (2.10)$$

Note that for all $i \geq 0$, Ξ_i is invariant under the operator L , and μ is an eigenvalue of L on Ξ_i if and only if it is an eigenvalue of the matrix $A - \lambda_i D$ for some $i \geq 0$, in which case, there exists an eigenvector in Ξ_i . Hence, we have an infinite number of ordinary differential systems with the second member $A - \lambda_i D$ for $i \in \mathbb{N}$. As a result, the zero solution of system (2.1)–(2.3) is asymptotically stable if for all $i \in \mathbb{N}$ the matrix $A - \lambda_i D$ satisfies the criterion of asymptotic stability in Theorem 2 of [69] and unstable if at least one matrix $A - \lambda_i D$ satisfies the instability criterion stated in the same theorem. ■

2.2.1.2 Incommensurate scenario

The next step is to identify the asymptotic stability conditions for system (2.1)–(2.3) when the fractional derivative orders α_k for $k = 1, \dots, N$ are not identical. We assume that the fractional orders $\alpha_k = \frac{l_k}{m_k} \in (0, 1]$ with $l_k, m_k \in \mathbb{N}$, and $\text{g.c.d.}(l_k, m_k) = 1$ for $k = 1, 2, \dots, N$. In addition, we let $m = \text{l.c.m.}\{m_1, \dots, m_N\}$ and $l = \text{g.c.d.}\{l_1, \dots, l_N\}$. It follows that for each pair (l_k, m_k) , there exist two positive integer numbers s_k and t_k such that $l_k = s_k l$ and $m_k = \frac{m}{t_k}$. By letting $\gamma = \frac{l}{m}$, we have $\alpha_k = q_k \gamma$, where $q_k = s_k t_k$ for $k = 1, \dots, N$ with the convention $q_0 = 0$. We also define:

$$\zeta_s^r := \sum_{i=0}^s q_i + r,$$

with $r, s \in \mathbb{N}_0$.

The following Lemma defines an important equivalence that is necessary for the proof of our main result.

Lemma 2.2.1. System (2.1)–(2.3) is equivalent to

$${}^C D_{0,t}^\gamma v_p(t, x) = \begin{cases} \Theta_k(A, D, v) & \text{if } p = \zeta_k^0, k = 1, \dots, N, \\ v_{p+1}(t, x) & \text{otherwise,} \end{cases} \quad (2.11)$$

where

$$\Theta_k(A, D, v) = d_k \Delta v_{\zeta_{k-1}^1}(t, x) + \sum_{j=1}^N a_{kj} v_{\zeta_{j-1}^1}(t, x),$$

subject to the initial conditions

$$v_p(0, x) = \begin{cases} u_k(0, x) & \text{if } p = \zeta_{k-1}^1, k = 1, \dots, N, \\ 0 & \text{otherwise,} \end{cases} \quad (2.12)$$

with $p = 1, \dots, \zeta_N^0$, and boundary conditions

$$(\mathbf{v} \cdot \nabla) v_{\zeta_{k-1}^1}(t, x) = 0, \quad t > 0, x \in \partial\Omega, \quad (2.13)$$

with $k = 1, \dots, N$.

Remark 2.2.1. The equivalence mentioned in Lemma 2.2.1 is in the following sense:

- Whenever $\left(v_1(t, x), v_2(t, x), \dots, v_{\zeta_N^0}(t, x)\right)^\top$ is the solution of system (2.11)–(2.13), the vector of functions

$$u(t, x) := \left(v_{\zeta_0^1}(t, x), v_{\zeta_1^1}(t, x), \dots, v_{\zeta_{N-1}^1}(t, x)\right)^\top,$$

solves the initial–boundary value problem (2.1)–(2.3).

- Whenever $u(t, x) = (u_1(t, x), \dots, u_N(t, x))^\top$ is the solution of the initial–boundary value problem (2.1)–(2.3), the vector function

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{q_1} \\ v_{q_1+1} \\ \vdots \\ v_{q_1+q_2} \\ \vdots \\ v_{q_1+\dots+q_{N-1}+1} \\ \vdots \\ v_{q_1+\dots+q_N} \end{pmatrix} := \begin{pmatrix} u_1 \\ {}^C D_{0,t}^Y u_1 \\ \vdots \\ {}^C D_{0,t}^{q_1 Y} u_1 \\ u_2 \\ \vdots \\ {}^C D_{0,t}^{q_2 Y} u_2 \\ \vdots \\ u_N \\ \vdots \\ {}^C D_{0,t}^{q_N Y} u_N \end{pmatrix}, \quad (2.14)$$

solves system (2.11)–(2.13).

Proof of Lemma 2.2.1. We introduce the ζ_N^0 functions $v_1, \dots, v_{\zeta_N^0}$, such that:

$$\left\{ \begin{array}{l} v_1(t, x) := u_1(t, x), \\ v_{\zeta_1^1}(t, x) := u_2(t, x), \\ \quad \quad \quad \vdots \\ v_{\zeta_{N-2}^1}(t, x) := u_{N-1}(t, x), \\ v_{\zeta_{N-1}^1}(t, x) := u_N(t, x). \end{array} \right. \quad (2.15)$$

By using the property 2 in Proposition 1.1.3, we can decompose the derivative operators ${}^C D_{0,t}^{\alpha_i}$ for $i = 1, \dots, N$ into a composition of q_i fractional derivative operators ${}^C D_{0,t}^Y$. Hence, equations (2.1) can be converted into the form:

$$\left\{ \begin{array}{l} {}^C D_{0,t}^Y v_1(t, x) = v_2(t, x), \\ {}^C D_{0,t}^Y v_2(t, x) = v_3(t, x), \\ \quad \quad \quad \vdots \\ {}^C D_{0,t}^Y v_{q_1-1}(t, x) = v_{q_1}(t, x), \\ {}^C D_{0,t}^Y v_{q_1}(t, x) = d_1 \Delta v_1(t, x) + \sum_{j=1}^N a_{1j} v_{\zeta_{j-1}^1}(t, x), \\ {}^C D_{0,t}^Y v_{q_1+1}(t, x) = v_{q_1+2}(t, x), \\ \quad \quad \quad \vdots \\ {}^C D_{0,t}^Y v_{q_1+q_2-1}(t, x) = v_{q_1+q_2}(t, x), \\ {}^C D_{0,t}^Y v_{q_1+q_2}(t, x) = d_2 \Delta v_{q_1+1}(t, x) + \sum_{j=1}^N a_{2j} v_{\zeta_{j-1}^1}(t, x), \\ {}^C D_{0,t}^Y v_{q_1+q_2+1}(t, x) = v_{q_1+q_2+2}(t, x), \\ \quad \quad \quad \vdots \\ {}^C D_{0,t}^Y v_{\zeta_N^0-1}(t, x) = v_{\zeta_N^0}(t, x), \\ {}^C D_{0,t}^Y v_{\zeta_N^0}(t, x) = d_N \Delta v_{\zeta_{N-1}^1}(t, x) + \sum_{j=1}^N a_{Nj} v_{\zeta_{j-1}^1}(t, x), \end{array} \right.$$

Before we present the stability criteria for the incommensurate case, let us define some new notations.

$$\mathcal{D} = \begin{pmatrix} \mathcal{D}_{11} & \mathcal{D}_{12} & \dots & \mathcal{D}_{1N} \\ \mathcal{D}_{21} & \mathcal{D}_{22} & \dots & \mathcal{D}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_{N1} & \mathcal{D}_{N2} & \dots & \mathcal{D}_{NN} \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \dots & \mathcal{A}_{1N} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \dots & \mathcal{A}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{A}_{N1} & \mathcal{A}_{N2} & \dots & \mathcal{A}_{NN} \end{pmatrix}.$$

The diagonal and off-diagonal submatrices \mathcal{D}_{ij} and \mathcal{A}_{ij} are defined differently as follows:

$$\mathcal{D}_{ii} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \\ d_i & 0 & \dots & 0 \end{pmatrix}_{q_i \times q_i}, \quad \mathcal{A}_{ii} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ a_{ii} & 0 & 0 & \dots & 0 \end{pmatrix}_{q_i \times q_i}, \quad i = 1, \dots, N,$$

and

$$\mathcal{D}_{ij} = \begin{pmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{pmatrix}_{q_i \times q_j}, \quad \mathcal{A}_{ij} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \\ a_{ij} & 0 & \dots & 0 \end{pmatrix}_{q_i \times q_j}, \quad i \neq j; i, j = 1, \dots, N.$$

Hence, the equations (2.11) can be rewritten in the form:

$${}^C D_{0,t}^Y v(t, x) = \mathcal{D}\Delta v(t, x) + \mathcal{A}v(t, x), \quad t > 0, \quad x \in \Omega, \quad (2.18)$$

where $v(x, t) = (v_1(t, x), v_2(t, x), \dots, v_{\zeta_N^0}(t, x))^\top$. Let $\tilde{v} := (\tilde{v}_1, \tilde{v}_2, \dots, \tilde{v}_{\zeta_N^0})$,

$$\mathcal{X} = \left\{ \tilde{v} \in [C(\bar{\Omega})]^{\zeta_N^0} \text{ and } \tilde{v}_{\zeta_{k-1}^1} \in C^2(\Omega) \mid (\nu \cdot \nabla) \tilde{v}_{\zeta_{k-1}^1} = 0, \text{ in } \partial\Omega, k = 1, \dots, N \right\},$$

$$\mathcal{X}_{ij} = \{c w_{ij} \mid c \in \mathbb{R}^{\zeta_N^0}\}, \text{ and } \mathcal{X}_i = \bigoplus_{j=1}^{m_i} \mathcal{X}_{ij}. \text{ This leads to the decomposition:}$$

$$\mathcal{X} = \bigoplus_{i=0}^{\infty} \mathcal{X}_i. \quad (2.19)$$

Finally, we define the operator $\mathcal{L} = \mathcal{D}\Delta + \mathcal{A}$. The following Theorem presents the stability criterion for the incommensurate case of (2.1)–(2.3).

Theorem 2.2.2. Suppose that the fractional orders are given by $\alpha_k = \frac{l_k}{m_k} \in (0, 1]$ with $l_k, m_k \in \mathbb{N}$, $\text{g.c.d.}(l_k, m_k) = 1$ for $k = 1, 2, \dots, N$ and let $m = \text{l.c.m.}\{m_1, \dots, m_N\}$. The zero solution of system (2.1)–(2.3) is asymptotically stable if both roots of equations

$$\det(\text{diag}(\xi^{m\alpha_1}, \dots, \xi^{m\alpha_N}) - A + \lambda_i D) = 0, \quad (2.20)$$

for all $i \in \mathbb{N}_0$ satisfy

$$|\arg(\xi)| > \frac{\pi}{2m}.$$

Alternatively, if at least one root of one equation from (2.20) satisfies $|\arg(\xi)| < \frac{\pi}{2m}$, then the zero solution of (2.1)–(2.3) is unstable.

Proof. The proof is straightforward thanks to the Lemma 2.2.1, which transforms the incommensurate time–fractional reaction–diffusion system (2.1)–(2.3) into the commensurate form (2.11)–(2.13). Since the two systems are equivalent in the sense of Remark 2.2.1, it suffices to guarantee the asymptotic stability of the second system. Consider the characteristic equation

$$\mathcal{L}(\Phi_1, \dots, \Phi_{\zeta_N^0})^\top = \mu(\Phi_1, \dots, \Phi_{\zeta_N^0})^\top, \quad (2.21)$$

where

$$(\Phi_1, \dots, \Phi_{\zeta_N^0})^\top = \sum_{i=0}^{\infty} \sum_{j=1}^{m_i} (\eta_{1ij}, \dots, \eta_{\zeta_N^0 ij})^\top w_{ij}. \quad (2.22)$$

This can be written more compactly as

$$\sum_{i=0}^{\infty} \sum_{j=1}^{m_i} (\mathcal{A} - \lambda_i \mathcal{D} - \mu I)(\eta_{1ij}, \dots, \eta_{\zeta_N^0 ij})^\top w_{ij} = 0. \quad (2.23)$$

For each $i \in \mathbb{N}_0$, we note that \mathcal{X}_i is invariant under operator \mathfrak{L} and that μ is an eigenvalue of \mathfrak{L} on \mathcal{X}_i iff it is an eigenvalue of the matrix $\mathcal{A} - \lambda_i \mathcal{D}$ for some $i \in \mathbb{N}_0$, in which case there exists an eigenvector in \mathcal{X}_i . As a result, we end up with an infinity of ODE systems with the second member $\mathcal{A} - \lambda_i \mathcal{D}$ for $i \in \mathbb{N}_0$ that depend on λ_i . Hence, it is well established that the zero solution of system (2.11)–(2.13) is asymptotically stable if the asymptotic stability condition stated in Theorem 2 of [69] is satisfied for all $i \in \mathbb{N}_0$, i.e. the roots of equations

$$\det(\mathcal{A} - \lambda_i \mathcal{D} - \mu \mathbf{I}) = 0,$$

satisfy $|\arg(\mu)| > \frac{\gamma\pi}{2}$.

Using the basic properties of the determinant, with $l = \text{g.c.d.}\{l_1, \dots, l_N\}$ then we obtain

$$\det(\mathcal{A} - \lambda_i \mathcal{D} - \xi^l \mathbf{I}) = 0 \iff \det(\text{diag}(\xi^{m\alpha_1}, \dots, \xi^{m\alpha_N}) - \mathbf{A} + \lambda_i \mathbf{D}) = 0,$$

leading to $|\arg(\xi)| > \frac{\pi}{2m}$. The second part of the Theorem regarding asymptotic instability can be proven using the same procedure. ■

2.2.2 Stability criteria for nonlinear fractional reaction–diffusion systems

In this section, we treat the more general nonlinear case. Consider the nonlinear time–fractional reaction diffusion system described by:

$${}^C D_{0,t}^{\hat{\alpha}} u(t, x) = D\Delta u(t, x) + F(u(t, x)), \quad t > 0, \quad x \in \Omega. \quad (2.24)$$

subject to initial states

$$u(0, x) = u_0(x), \quad x \in \Omega, \quad (2.25)$$

and Neumann boundary conditions

$$(\mathbf{v} \cdot \nabla) u(t, x) = 0, \quad t > 0, \quad x \in \partial\Omega. \quad (2.26)$$

In this case, $F(u(t, x)) = (F_1(u(t, x)), \dots, F_N(u(t, x)))^\top$ is a nonlinear function in C^2 . The following definition describes the constant (or homogeneous) steady–state solution of that nonlinear system.

Definition 2.2.1. The constant vector u_{eq} is said to be a constant steady-state solution of (2.24) subject to the initial data (2.25) and homogeneous Neumann boundary conditions (2.26) iff $F(u_{eq}) = 0$.

In order to simplify the calculations, we transform our system to one with zero as its steady state. We introduce the translation $u(t, x) = \vartheta(t, x) + u_{eq}$ where $\vartheta(t, x) =$

$(\vartheta_1(t, x), \dots, \vartheta_N(t, x))^\top$ and u_{eq} denotes the homogeneous steady–state solution of system (2.24)–(2.26). Since the Caputo derivative of a constant is equal to zero, we end up with

$${}^C D_{0,t}^{\hat{\alpha}} \vartheta(t, x) = D\Delta\vartheta(t, x) + F(\vartheta(t, x) + u_{eq}). \quad (2.27)$$

The nonlinear function F can be linearized by means of its Taylor series expansion around the steady–state u_{eq} leading to

$$F(\vartheta(t, x) + u_{eq}) = F(u_{eq}) + J|_{u_{eq}} \vartheta(t, x) + \mathcal{O}(\|\vartheta(t, x)\|^2),$$

where

$$J|_{u_{eq}} = \left(\frac{\partial F_i(u_{eq})}{\partial u_j} \right)_{1 \leq i, j \leq N},$$

is the Jacobian matrix corresponding to F . Ignoring higher terms, we obtain the approximation

$$F(\vartheta(t, x) + u_{eq}) \approx J|_{u_{eq}} \vartheta(t, x).$$

Therefore, the linearized version of the system is simply

$${}^C D_{0,t}^{\hat{\alpha}} \vartheta(t, x) = D\Delta\vartheta(t, x) + J|_{u_{eq}} \vartheta(t, x), \quad t > 0, \quad x \in \Omega, \quad (2.28)$$

with the initial and boundary conditions

$$\vartheta(0, x) = \vartheta_0(x), \quad x \in \Omega, \quad (2.29)$$

$$(\mathbf{v} \cdot \nabla) \vartheta(t, x) = 0, \quad t > 0, \quad x \in \partial\Omega. \quad (2.30)$$

Corollary 2.2.1. Subject to the identical fractional–orders $\alpha_1 = \dots = \alpha_N = \alpha \in (0, 1]$, the steady–state u_{eq} of system (2.24)–(2.26) is asymptotically stable if both roots of

$$\det(J|_{u_{eq}} - \lambda_i D - \mu I) = 0, \quad (2.31)$$

satisfy $|\arg(\mu)| > \frac{\alpha\pi}{2}$ for all $i \in \mathbb{N}_0$. Alternatively, if at least one root of one equation satisfies $|\arg(\mu)| < \frac{\alpha\pi}{2}$, then u_{eq} is unstable.

Proof. Theorem 2.2.1 can be applied directly to the linearized system (2.28)–(2.30) at the constant steady–state solution u_{eq} . ■

Corollary 2.2.2. Subject to the non–identical fractional orders $\alpha_k = \frac{l_k}{m_k} \in (0, 1]$ with $l_k, m_k \in \mathbb{N}$, where $\text{g.c.d.}(l_k, m_k) = 1$ for $k = 1, 2, \dots, N$ and $m = \text{l.c.m.}\{m_1, \dots, m_N\}$,

the constant steady-state u_{eq} of system (2.24)–(2.26) is asymptotically stable if both the roots of equations

$$\det(\text{diag}(\xi^{m\alpha_1}, \dots, \xi^{m\alpha_N}) - J|_{u_{eq}} + \lambda_i D) = 0, \quad i \in \mathbb{N}_0, \quad (2.32)$$

satisfy $|\arg(\xi)| > \frac{\pi}{2m}$. Alternatively, if at least one root of one equation satisfies $|\arg(\xi)| < \frac{\pi}{2m}$, then u_{eq} becomes unstable.

Proof. This result follows directly from Theorem 2.2.2 when considering the linearized system (2.28)–(2.30) at the constant steady-state u_{eq} . ■

2.3 Examples and numerical experiments

In order to validate and illustrate the theoretical stability criteria proposed in this paper for linear and nonlinear time-fractional reaction-diffusion systems, we resort to some numerical examples. We consider two specific examples: the Schnackenberg model proposed in [114] and the Gause-type predator-prey model examined in [115]. Numerical solutions in one-dimensional space are obtained by means of the numerical scheme proposed in [21] with time step $h_t = 0.0625$ and spatial step $h_x = 0.2$. In the following, we discuss the solutions and asymptotic stability of these two models subject to different parameter sets.

Example 2.3.1. We start with the Schnackenberg nonlinear model [114], which is described by

$$\left\{ \begin{array}{ll} {}^C D_{0,t}^{\alpha_1} u_1 = d_1 \Delta u_1 + a - u_1 + u_1^2 u_2 & \text{in } (0, \infty) \times \Omega, \\ {}^C D_{0,t}^{\alpha_2} u_2 = d_2 \Delta u_2 + b - u_1^2 u_2 & \text{in } (0, \infty) \times \Omega, \\ u_1(0, x) = u_{1,0}(x), u_2(0, x) = u_{2,0}(x) & \text{on } \Omega, \\ (\mathbf{v} \cdot \nabla) u_1(t, x) = (\mathbf{v} \cdot \nabla) u_2(t, x) = 0, & \text{on } (0, \infty) \times \partial\Omega, \end{array} \right. \quad (2.33)$$

where $\alpha_1, \alpha_2 \in (0, 1]$ and $a, b, d_1, d_2 > 0$. System (2.33) has the unique steady state

$$E_{st} = \left(a + b, \frac{b}{(a + b)^2} \right).$$

By linearizing (2.33) at E_{st} , we obtain the linear system

$$\left\{ \begin{array}{ll} {}^C D_{0,t}^{\alpha_1} u_1 = d_1 \Delta u_1 + \left(\frac{2b}{a+b} - 1 \right) u_1 + (a+b)^2 u_2 & \text{in } (0, \infty) \times \Omega, \\ {}^C D_{0,t}^{\alpha_2} u_2 = d_2 \Delta u_2 - \frac{2b}{a+b} u_1 - (a+b)^2 u_2 & \text{in } (0, \infty) \times \Omega, \\ u_1(0, x) = u_{1,0}(x), u_2(0, x) = u_{2,0}(x) & \text{on } \Omega, \\ (\mathbf{v} \cdot \nabla) u_1(t, x) = (\mathbf{v} \cdot \nabla) u_2(t, x) = 0, & \text{on } (0, \infty) \times \partial\Omega. \end{array} \right. \quad (2.34)$$

We assume the initial conditions

$$\left\{ \begin{array}{l} u_{1,0}(x) = 0.68 + \frac{\cos(x)}{10}, \\ u_{2,0}(x) = 0.78 + \frac{\sin(x)}{10}. \end{array} \right.$$

In order to assess the validity of the theoretical stability criteria derived earlier, let us consider the following sets of parameters:

1. Let $\Omega = (0, 10)$, $(\alpha_1, \alpha_2) = (\sqrt{\frac{5}{9}}, \sqrt{\frac{5}{9}})$, and $(a, b, d_1, d_2) = (0.14, 0.54, 0.02, 0.01)$. Using Theorem 1, we conclude that the zero solution of system (2.34) is asymptotically stable. The numerical solutions depicted in Figure 2.1 agree with the theoretical results. By Corollary 1, it follows that the unique steady–state $E_{st} = (0.68, 1.1678)$ of system (2.33) is asymptotically stable, which again agrees with the results in Figure 2.2.
2. Let $\Omega = (0, 10)$, $(\alpha_1, \alpha_2) = (\frac{1}{3}, \frac{1}{2})$, and $(a, b, d_1, d_2) = (0.14, 0.54, 0.02, 0.01)$. Using Corollary 2, we know that the steady–state $E_{st} = (0.68, 1.1678)$ of system (2.33) is asymptotically stable. The numerical solutions are depicted in Figure 2.3.
3. Let $\Omega = (0, 10)$, $(\alpha_1, \alpha_2) = (\frac{6}{9}, \frac{7}{8})$, and $(a, b, d_1, d_2) = (0.042, 0.626, 0.02, 0.01)$. Using Theorem 2, we conclude that the zero steady–state of system (2.34) is asymptotically stable, and consequently, by Corollary (2), the steady–state $E_{st} = (0.668, 1.4029)$ of system (2.33) is also asymptotically stable. The numerical solutions of systems (2.33) and (2.34) are depicted, respectively, in Figures 2.4 and 2.5.
4. Let $\Omega = (0, 10)$, $(\alpha_1, \alpha_2) = (\frac{9}{10}, \frac{8}{10})$, and $(a, b, d_1, d_2) = (0.042, 0.626, 0.02, 0.01)$. By Corollary (2), system (2.33) is unstable, which agrees with the numerical solutions in Figure 2.6.

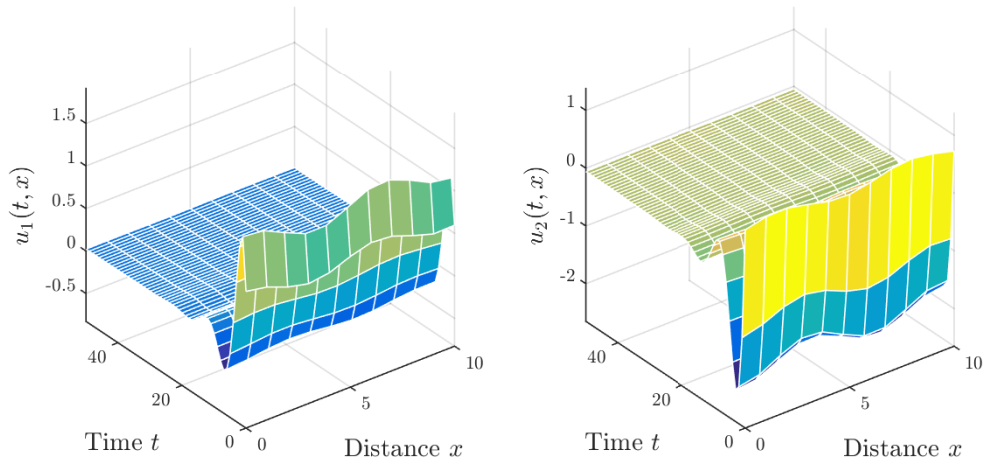


Figure 2.1: Numerical solutions of system (2.34) subject to the first set of parameters.

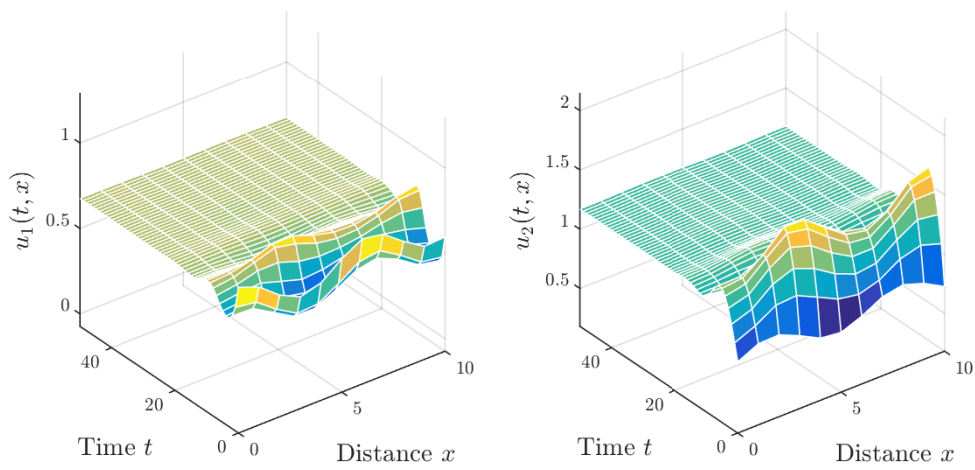


Figure 2.2: Numerical solutions of system (2.33) subject to the first set of parameters.

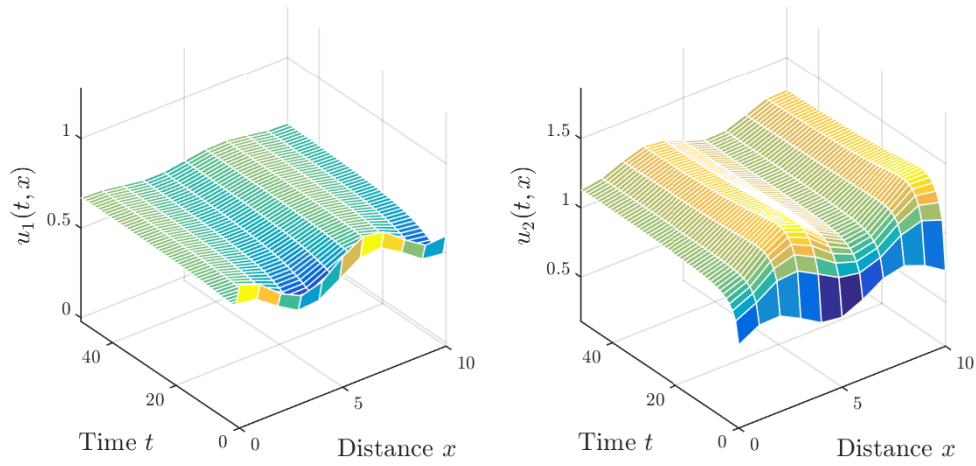


Figure 2.3: Numerical solutions of system (2.33) subject to the second set of parameters.

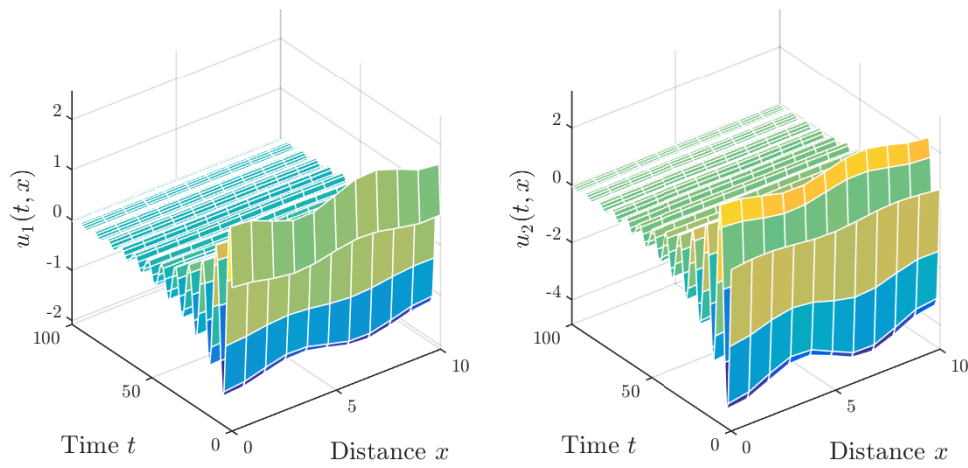


Figure 2.4: Numerical solutions of system (2.34) subject to the third set of parameters.

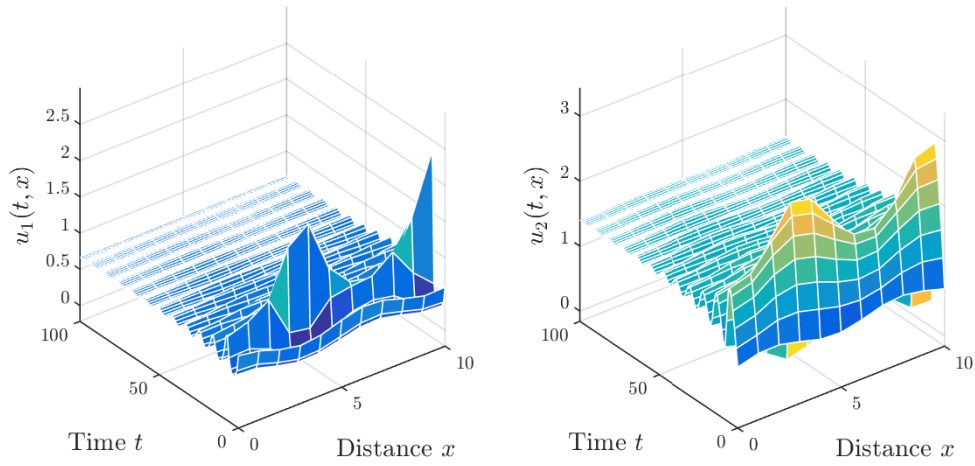


Figure 2.5: Numerical solutions of system (2.33) subject to the third set of parameters.

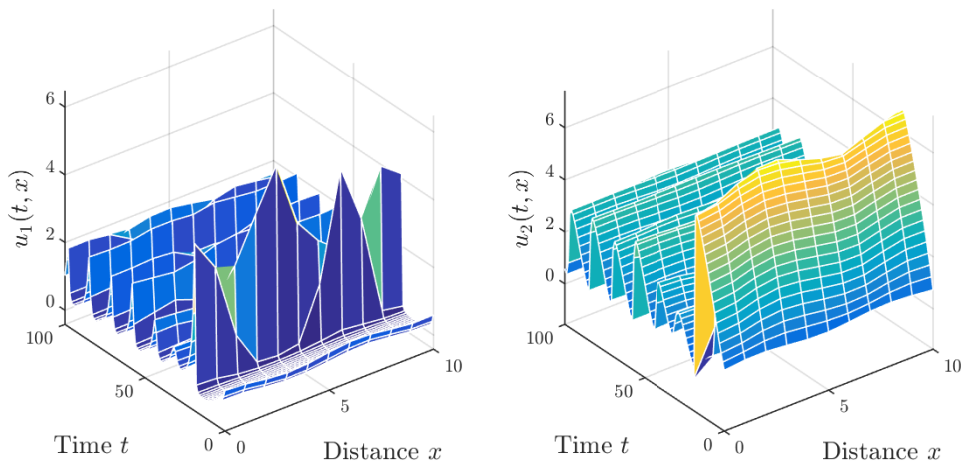


Figure 2.6: Numerical solutions of system (2.33) subject to the fourth set of parameters.

Example 2.3.2. Our second example is the Gause–type predator–prey model discussed in [115], which is of the form

$$\left\{ \begin{array}{ll} {}^C D_{0,t}^{\alpha_1} u_1 = d_1 \Delta u_1 + r u_1 (1 - u_1) - u_2 \sqrt{u_1} & \text{in } (0, \infty) \times \Omega, \\ {}^C D_{0,t}^{\alpha_2} u_2 = d_2 \Delta u_2 + \beta u_2 (\sqrt{u_1} - \delta) & \text{in } (0, \infty) \times \Omega, \\ u_1(0, x) = u_{1,0}(x), u_2(0, x) = u_{2,0}(x) & \text{on } \Omega, \\ (\mathbf{v} \cdot \nabla) u_1(t, x) = (\mathbf{v} \cdot \nabla) u_2(t, x) = 0, & \text{on } (0, \infty) \times \partial\Omega, \end{array} \right. \quad (2.35)$$

where $\alpha_1, \alpha_2 \in (0, 1]$ and $r, \beta, \delta, d_1, d_2 > 0$. As shown in [115], system (2.35) has the three steady–states $E_0 = (0, 0)$, $E_1 = (1, 0)$, and $E_2 = (\delta^2, r\delta(1 - \delta^2))$. In our simulations, we assume the initial conditions

$$\left\{ \begin{array}{l} u_{1,0}(x) = 0.047 + \frac{\cos(x)}{10}, \\ u_{2,0}(x) = 0.083 + \frac{\sin(x)}{10}. \end{array} \right.$$

We consider three sets of parameters:

1. Let $\Omega = (0, 1)$, $(\alpha_1, \alpha_2) = (\sqrt{\frac{4}{7}}, \sqrt{\frac{4}{7}})$, and $(r, \beta, \delta, d_1, d_2) = (0.5, 0.7, 0.6, 1, 0.3)$. Corollary (1) tells us that the steady–state $E_2 = (0.36, 0.192)$ of system (2.35) is asymptotically stable, which agrees with the numerical solution in Figure 2.7.
2. Let $\Omega = (0, 1)$, $(\alpha_1, \alpha_2) = (\frac{3}{5}, \frac{2}{3})$, and $(r, \beta, \delta, d_1, d_2) = (0.5, 0.7, 0.6, 1, 0.3)$. From Corollary (2), we see that the steady–state $E_2 = (0.36, 0.192)$ is asymptotically stable. Again, this agrees with the results in Figure 2.8.
3. Let $\Omega = (0, 1)$, $(\alpha_1, \alpha_2) = (\frac{5}{6}, \frac{7}{8})$, and $(r, \beta, \delta, d_1, d_2) = (0.5, 0.7, 0.3, 1, 0.3)$. Using Corollary (2), we find that none of the steady–states are asymptotically stable. Indeed, the numerical solution depicted in Figure 2.9 seems to be periodic in nature.

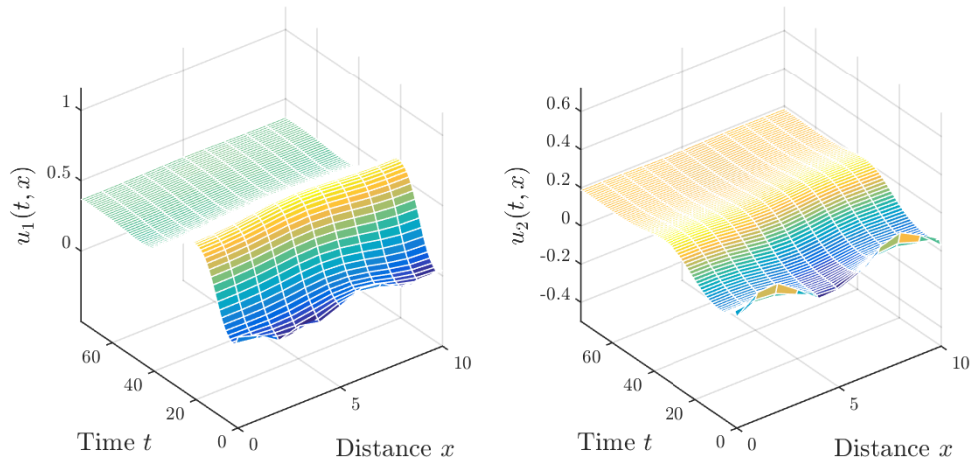


Figure 2.7: Numerical solutions of system (2.35) subject to the first set of parameters.

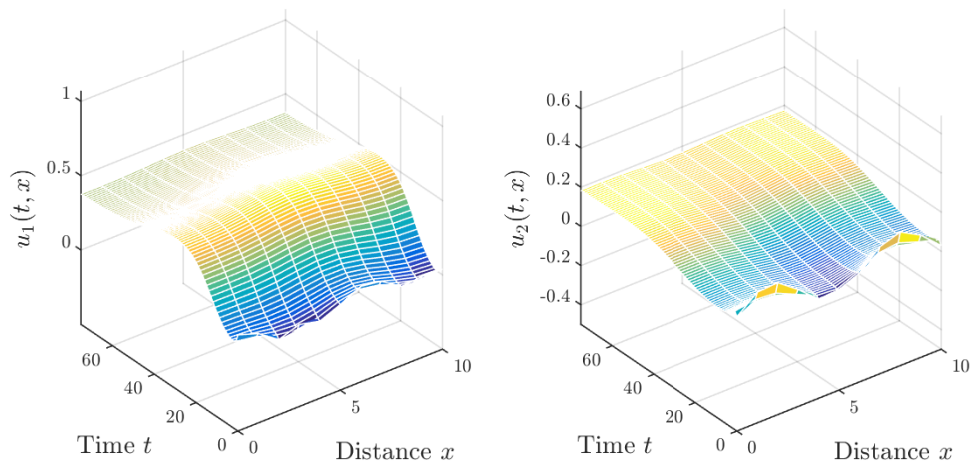


Figure 2.8: Numerical solutions of system (2.35) subject to the second set of parameters.

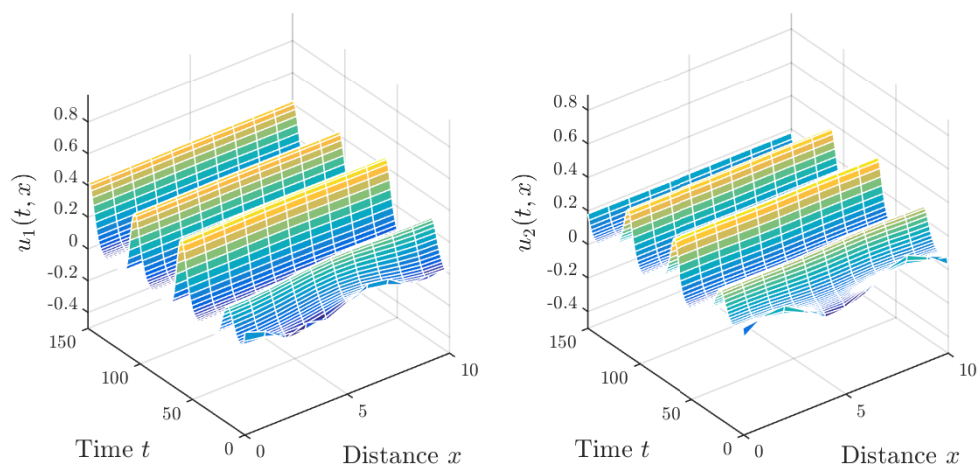


Figure 2.9: Numerical solutions of system (2.35) subject to the third set of parameters.

CHAPTER

3

NUMERICAL METHODS FOR TIME-FRACTIONAL REACTION-DIFFUSION/ODE SYSTEMS

In a reply letter to Leibniz in 1695, L'Hôpital asked: "What if the order of derivative will be $\frac{1}{2}$?"
Leibniz in a letter dated September 30, 1695 - the exact birthday of the fractional calculus! - replied: "It will lead to a paradox, from which one day useful consequences will be drawn."

Leibniz & L'Hôpital

This chapter is a continuation and support to the previous chapter, where an efficient numerical method is derived for solving time-fractional reaction-diffusion systems. The proposed numerical scheme is the method of lines (MOL), which depends on solving fractional differential systems. The results appearing in this context have been published through [30, 34].

In the first two sections, we made several improvements to the predictor-corrector method, relying on Newton's and Lagrange's interpolation, and we tested the effectiveness and performance of these proposed methods on several examples.

3.1 A Newton interpolation based predictor-corrector numerical method for fractional differential equations

This section presents a new predictor-corrector numerical scheme suitable for fractional differential equations. An improved explicit Atangana-Seda formula is obtained by considering the neglected terms and used as the predictor stage of the proposed method. Numerical formulas are presented that approximate the classical first derivative as well as the Caputo, Caputo-Fabrizio and Atangana-Baleanu fractional derivatives. Simulation results are used to assess the approximation error of the new method for various differential equations. In addition, a case study is considered where the proposed scheme is used to obtain numerical solutions of the Gierer-Meinhardt activator-inhibitor model with the aim of assessing the system's dynamics.

3.1.1 The proposed predictor-corrector method

3.1.1.1 Classical derivative

We start with the simple classical initial-value problem given by

$$\begin{cases} \frac{dy(t)}{dt} = f(t, y(t)), \\ y(0) = y_0, \end{cases} \quad (3.1)$$

where f is a smooth nonlinear function guaranteeing a unique solution $y(t)$. In order to develop a numerical formula approximating the solution of (3.1), we convert the differential equation into the integral

$$y(t) - y(0) = \int_0^t f(s, y(s)) ds. \quad (3.2)$$

In an iterative approximation, we may choose two distinct points in time $t_m = m\Delta t$ and $t_{m+1} = (m+1)\Delta t$. Substituting these points into (3.2) yields

$$y(t_m) - y(0) = \int_0^{t_m} f(s, y(s)) ds,$$

and

$$y(t_{m+1}) - y(0) = \int_0^{t_{m+1}} f(s, y(s)) ds,$$

respectively. Taking the difference yields

$$y(t_{m+1}) - y(t_m) = \int_{t_m}^{t_{m+1}} f(s, y(s)) ds. \quad (3.3)$$

Hence, the function $f(s, y(s))$ may be approximated over the interval $[t_m, t_{m+1}]$ by means of Newton's second order interpolation polynomial given by

$$\begin{aligned} \mathcal{N}_m(s) &= f(t_{m+1}, y(t_{m+1})) + \frac{f(t_{m+1}, y(t_{m+1})) - f(t_m, y(t_m))}{\Delta t} (s - t_{m+1}) \\ &\quad + \frac{f(t_{m+1}, y(t_{m+1})) - 2f(t_m, y(t_m)) + f(t_{m-1}, y(t_{m-1}))}{2(\Delta t)^2} \\ &\quad \times (s - t_m)(s - t_{m+1}). \end{aligned} \quad (3.4)$$

Substitution into (3.3) leads to the difference formula

$$\begin{aligned} y_{m+1} - y_m &= f(t_{m+1}, y_{m+1}) \Delta t + \left(\frac{f(t_{m+1}, y_{m+1}) - f(t_m, y_m)}{\Delta t} \right) \int_{t_m}^{t_{m+1}} (s - t_{m+1}) ds \\ &\quad + \left(\frac{f(t_{m+1}, y_{m+1}) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})}{2(\Delta t)^2} \right) \\ &\quad \int_{t_m}^{t_{m+1}} (s - t_m)(s - t_{m+1}) ds. \end{aligned} \quad (3.5)$$

Given that

$$\int_{t_m}^{t_{m+1}} (s - t_{m+1}) ds = -\frac{(\Delta t)^2}{2}, \quad (3.6)$$

and

$$\int_{t_m}^{t_{m+1}} (s - t_m)(s - t_{m+1}) ds = -\frac{(\Delta t)^3}{6}, \quad (3.7)$$

formula (3.5) reduces to the implicit form

$$\begin{aligned} y_{m+1} - y_m &= f(t_{m+1}, y_{m+1}) \Delta t - [f(t_{m+1}, y_{m+1}) - f(t_m, y_m)] \frac{\Delta t}{2} \\ &\quad - [f(t_{m+1}, y_{m+1}) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})] \frac{\Delta t}{12}. \end{aligned} \quad (3.8)$$

The term y_{m+1} appears on both sides of the formula. The predictor-corrector scheme works by first producing an approximation of y_{m+1} denoted by y_{m+1}^P , and then using (3.8) to correct the approximation. The correction formula is, thus, given by (it is the same the two step Adams-Moulton scheme)

$$y_{m+1} = y_m + \frac{5}{12} f(t_{m+1}, y_{m+1}^P) \Delta t + \frac{2}{3} f(t_m, y_m) \Delta t - f(t_{m-1}, y_{m-1}) \frac{\Delta t}{12}, \quad (3.9)$$

where the predictor y_{m+1}^p is obtained by means of the Atangana-Seda scheme (two step Adams-Moulton method), it is the same the three step Adams-Bashforth method (cf. [9] and [14, p. 110]), i.e.

$$y_{m+1}^p = y_m + \frac{5}{12}f(t_{m-2}, y_{m-2})\Delta t - \frac{4}{3}f(t_{m-1}, y_{m-1})\Delta t + \frac{23}{12}f(t_m, y_m)\Delta t. \quad (3.10)$$

Throughout the remainder, We deal with various fractional derivatives.

3.1.1.2 Caputo fractional derivative

The most commonly fractional derivative used is the so-called Caputo fractional derivative one. We consider the initial-value problem:

$$\begin{cases} {}_0^C D_t^\alpha y(t) = f(t, y(t)), \\ y(0) = y_0, \end{cases} \quad (3.11)$$

with $\alpha \in (0, 1]$, and f being a smooth nonlinear function such that (3.11) admits a unique solution $y(t)$. Following the same procedure of the standard case, we start with the integral

$$y(t) - y(0) = \frac{1}{\Gamma(\alpha)} \int_0^t f(s, y(s))(t-s)^{\alpha-1} ds. \quad (3.12)$$

Note that we have applied the left-sided α -order Riemann-Liouville fractional integral to both sides of the Caputo fractional differential equation, i.e. the first equation of (3.11), and incorporated the initial condition (cf. [27]). At the single point $t_{m+1} = (m+1)\Delta t$, we have

$$\begin{aligned} y(t_{m+1}) &= y(0) + \frac{1}{\Gamma(\alpha)} \int_0^{t_{m+1}} f(s, y(s))(t_{m+1}-s)^{\alpha-1} ds \\ &= y(0) + \frac{1}{\Gamma(\alpha)} \sum_{i=0}^m \int_{t_i}^{t_{i+1}} f(s, y(s))(t_{m+1}-s)^{\alpha-1} ds, \end{aligned} \quad (3.13)$$

with $t_0 = 0$. Function $f(s, y(s))$ can be approximated over the sub-interval $[t_i, t_{i+1}]$ as a polynomial by means of

$$\mathcal{N}_i(s) = \begin{cases} \widetilde{\mathcal{N}}_i(s) & \text{if } i = 0, \\ \widehat{\mathcal{N}}_i(s) & \text{if } i \in \{1, \dots, m\}, \end{cases} \quad (3.14)$$

where

$$\widetilde{\mathcal{N}}_i(s) = f(t_i, y(t_i)) + \left(\frac{f(t_{i+1}, y(t_{i+1})) - f(t_i, y(t_i))}{\Delta t} \right) (s - t_i), \quad (3.15)$$

and

$$\begin{aligned} \widehat{\mathcal{N}}_i(s) = & f(t_{i+1}, y(t_{i+1})) + \frac{f(t_{i+1}, y(t_{i+1})) - f(t_i, y(t_i))}{\Delta t} (s - t_{i+1}) \\ & + \frac{f(t_{i+1}, y(t_{i+1})) - 2f(t_i, y(t_i)) + f(t_{i-1}, y(t_{i-1}))}{2(\Delta t)^2} \\ & \times (s - t_i)(s - t_{i+1}). \end{aligned} \quad (3.16)$$

Using the Newton polynomial (4.108), formula (3.13) becomes

$$\begin{aligned} y(t_{m+1}) = & y(0) + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} \left[f(t_0, y(t_0)) + \left(\frac{f(t_1, y(t_1)) - f(t_0, y(t_0))}{\Delta t} \right) s \right] (t_{m+1} - s)^{\alpha-1} ds \\ & + \frac{1}{\Gamma(\alpha)} \\ & \sum_{i=1}^m \int_{t_i}^{t_{i+1}} \left\{ \begin{array}{l} f(t_{i+1}, y(t_{i+1})) \\ + \frac{f(t_{i+1}, y(t_{i+1})) - f(t_i, y(t_i))}{\Delta t} (s - t_{i+1}) \\ + \frac{f(t_{i+1}, y(t_{i+1})) - 2f(t_i, y(t_i)) + f(t_{i-1}, y(t_{i-1}))}{2(\Delta t)^2} \\ \times (s - t_i)(s - t_{i+1}) \end{array} \right\} (t_{m+1} - s)^{\alpha-1} ds. \end{aligned} \quad (3.17)$$

Simplifying and rearranging the terms leads to

$$\begin{aligned} y_{m+1} = & y_0 + \frac{1}{\Gamma(\alpha)} f(t_0, y_0) \int_0^{t_1} (t_{m+1} - s)^{\alpha-1} ds + \frac{1}{\Gamma(\alpha)} \left(\frac{f(t_1, y_1) - f(t_0, y_0)}{\Delta t} \right) \int_0^{t_1} s (t_{m+1} - s)^{\alpha-1} ds \\ & + \frac{1}{\Gamma(\alpha)} \sum_{i=1}^m f(t_{i+1}, y_{i+1}) \int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds \\ & + \frac{1}{\Gamma(\alpha)} \sum_{i=1}^m \frac{f(t_{i+1}, y_{i+1}) - f(t_i, y_i)}{\Delta t} \int_{t_i}^{t_{i+1}} (s - t_{i+1}) (t_{m+1} - s)^{\alpha-1} ds \\ & + \frac{1}{\Gamma(\alpha)} \sum_{i=1}^m \frac{f(t_{i+1}, y_{i+1}) - 2f(t_i, y_i) + f(t_{i-1}, y_{i-1})}{2(\Delta t)^2} \\ & \times \int_{t_i}^{t_{i+1}} (s - t_i)(s - t_{i+1}) (t_{m+1} - s)^{\alpha-1} ds. \end{aligned} \quad (3.18)$$

The four different integrals in (3.18) can be calculated as

$$\int_0^{t_1} s (t_{m+1} - s)^{\alpha-1} ds = \frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)} [(m+1)^{\alpha+1} - m^{\alpha+1} - (\alpha+1)m^\alpha], \quad (3.19)$$

$$\int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds = \frac{(\Delta t)^\alpha}{\alpha} [(m-i+1)^\alpha - (m-i)^\alpha], \quad (3.20)$$

$$\int_{t_i}^{t_{i+1}} (s - t_{i+1})(t_{m+1} - s)^{\alpha-1} ds = \frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)} [(m-i-\alpha)(m-i+1)^\alpha - (m-i)^{\alpha+1}], \quad (3.21)$$

and

$$\int_{t_i}^{t_{i+1}} (s - t_i)(s - t_{i+1})(t_{m+1} - s)^{\alpha-1} ds = \begin{bmatrix} (m-i+1)^\alpha \begin{bmatrix} 2(m-i)^2 - \alpha(m-i+1) \\ +2(m-i) \end{bmatrix} \\ -(m-i)^\alpha \begin{bmatrix} 2(m-i)^2 + \alpha(m-i) \\ +2(m-i) \end{bmatrix} \end{bmatrix} \times \frac{(\Delta t)^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}, \quad (3.22)$$

respectively. By substituting these calculations into (3.18), we obtain

$$\begin{aligned} y_{m+1} = & y_0 + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} f(t_0, y_0) [(m+1)^\alpha - m^\alpha] \\ & + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} (f(t_1, y_1) - f(t_0, y_0)) [(m+1)^{\alpha+1} - m^{\alpha+1} - (\alpha+1)m^\alpha] \\ & + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} \sum_{i=1}^m f(t_{i+1}, y_{i+1}) [(m-i+1)^\alpha - (m-i)^\alpha] \\ & + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \sum_{i=1}^m (f(t_{i+1}, y_{i+1}) - f(t_i, y_i)) [(m-i-\alpha)(m-i+1)^\alpha - (m-i)^{\alpha+1}] \\ & + \frac{(\Delta t)^\alpha}{2\Gamma(\alpha+3)} \sum_{i=1}^m (f(t_{i+1}, y_{i+1}) - 2f(t_i, y_i) + f(t_{i-1}, y_{i-1})) \\ & \times \begin{bmatrix} (m-i+1)^\alpha \begin{bmatrix} 2(m-i)^2 - \alpha(m-i+1) \\ +2(m-i) \end{bmatrix} \\ -(m-i)^\alpha \begin{bmatrix} 2(m-i)^2 + \alpha(m-i) \\ +2(m-i) \end{bmatrix} \end{bmatrix}. \end{aligned} \quad (3.23)$$

In order to simplify the formulas to come, let us define the expression

$$\begin{aligned}
 Y_p &= \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} \sum_{i=1}^p f(t_{i+1}, y_{i+1}) [(m-i+1)^\alpha - (m-i)^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \sum_{i=1}^p (f(t_{i+1}, y_{i+1}) - f(t_i, y_i)) [(m-i-\alpha)(m-i+1)^\alpha - (m-i)^{\alpha+1}] \\
 &+ \frac{(\Delta t)^\alpha}{2\Gamma(\alpha+3)} \sum_{i=1}^p (f(t_{i+1}, y_{i+1}) - 2f(t_i, y_i) + f(t_{i-1}, y_{i-1})) \\
 &\quad \times \begin{bmatrix} (m-i+1)^\alpha \begin{bmatrix} 2(m-i)^2 - \alpha(m-i+1) \\ +2(m-i) \end{bmatrix} \\ -(m-i)^\alpha \begin{bmatrix} 2(m-i)^2 + \alpha(m-i) \\ +2(m-i) \end{bmatrix} \end{bmatrix}, \tag{3.24}
 \end{aligned}$$

with the convention

$$Y_0 = 0. \tag{3.25}$$

Using this notation, (3.23) can be rewritten in the form

$$\begin{aligned}
 y_{m+1} &= y_0 + Y_{m-1} + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} f(t_0, y_0) [(m+1)^\alpha - m^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} (f(t_1, y_1) - f(t_0, y_0)) [(m+1)^{\alpha+1} - m^{\alpha+1} - (\alpha+1)m^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} f(t_{m+1}, y_{m+1}) + \frac{\alpha(\Delta t)^\alpha}{\Gamma(\alpha+2)} (f(t_m, y_m) - f(t_{m+1}, y_{m+1})) \\
 &- \frac{\alpha(\Delta t)^\alpha}{2\Gamma(\alpha+3)} (f(t_{m+1}, y_{m+1}) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})). \tag{3.26}
 \end{aligned}$$

Formula (3.26) will serve as our implicit part, i.e. the corrector. The terms y_{m+1} on the right hand side will be replaced by the predictor y_{m+1}^P , which will be an improved version of the Atangana-Seda scheme derived for the Caputo fractional derivative in [8]. To obtain our predictor formula, let us go back to (3.12) and use the predictor notation $y^P(t)$, which yields

$$y^P(t) - y(0) = \frac{1}{\Gamma(\alpha)} \int_0^t f(s, y(s))(t-s)^{\alpha-1} ds,$$

and, consequently, at $t_{m+1} = (m+1)\Delta t$, we have

$$y^P(t_{m+1}) = y(0) + \frac{1}{\Gamma(\alpha)} \sum_{i=0}^m \int_{t_i}^{t_{i+1}} f(s, y(s))(t_{m+1}-s)^{\alpha-1} ds. \tag{3.27}$$

The function $f(s, y(s))$ can be approximated over each sub-interval $[t_i, t_{i+1}]$ using a delayed version of the Newton's polynomial seen earlier, given by

$$\mathcal{N}_i^{\text{P}}(s) = \begin{cases} \widetilde{\mathcal{N}}_i^{\text{P}}(s) & \text{if } i \in \{0, 1\}, \\ \widehat{\mathcal{N}}_i^{\text{P}}(s) & \text{if } i \in \{2, \dots, m\}, \end{cases} \quad (3.28)$$

where

$$\widetilde{\mathcal{N}}_i^{\text{P}}(s) = f(t_i, y(t_i)) + \left(\frac{f(t_{i+1}, y(t_{i+1})) - f(t_i, y(t_i))}{\Delta t} \right) (s - t_i), \quad (3.29)$$

and

$$\begin{aligned} \widehat{\mathcal{N}}_i^{\text{P}}(s) &= f(t_{i-2}, y(t_{i-2})) + \left(\frac{f(t_{i-1}, y(t_{i-1})) - f(t_{i-2}, y(t_{i-2}))}{\Delta t} \right) (s - t_{i-2}) \\ &\quad + \left(\frac{f(t_i, y(t_i)) - 2f(t_{i-1}, y(t_{i-1})) + f(t_{i-2}, y(t_{i-2}))}{2(\Delta t)^2} \right) \\ &\quad \times (s - t_{i-2})(s - t_{i-1}). \end{aligned} \quad (3.30)$$

Substituting the interpolated approximation of $f(s, y(s))$ into (3.27) yields the predictor

$$\begin{aligned} y_{m+1}^{\text{P}} &= y_0 + \frac{1}{\Gamma(\alpha)} \sum_{i=0}^1 f(t_i, y_i) \int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds \\ &\quad + \frac{1}{\Gamma(\alpha)} \sum_{i=0}^1 \frac{f(t_{i+1}, y_{i+1}) - f(t_i, y_i)}{\Delta t} \int_{t_i}^{t_{i+1}} (s - t_i) (t_{m+1} - s)^{\alpha-1} ds \\ &\quad + \frac{1}{\Gamma(\alpha)} \sum_{i=2}^m f(t_{i-2}, y_{i-2}) \int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds \\ &\quad + \frac{1}{\Gamma(\alpha)} \sum_{i=2}^m \frac{f(t_{i-1}, y_{i-1}) - f(t_{i-2}, y_{i-2})}{\Delta t} \int_{t_i}^{t_{i+1}} (s - t_{i-2}) (t_{m+1} - s)^{\alpha-1} ds \\ &\quad + \frac{1}{\Gamma(\alpha)} \sum_{i=2}^m \frac{f(t_i, y_i) - 2f(t_{i-1}, y_{i-1}) + f(t_{i-2}, y_{i-2})}{2(\Delta t)^2} \\ &\quad \times \int_{t_i}^{t_{i+1}} (s - t_{i-2})(s - t_{i-1}) (t_{m+1} - s)^{\alpha-1} ds. \end{aligned} \quad (3.31)$$

We can calculate the integrals as

$$\int_{t_i}^{t_{i+1}} (s - t_i) (t_{m+1} - s)^{\alpha-1} ds = \frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)} \left[(m-i+1)^{\alpha+1} - (m-i)^{\alpha+1} - (\alpha+1)(m-i)^{\alpha} \right], \quad (3.32)$$

$$\int_{t_i}^{t_{i+1}} (s - t_{i-2})(t_{m+1} - s)^{\alpha-1} ds = \frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)} \begin{bmatrix} (m-i+1)^\alpha(m-i+3+2\alpha) \\ -(m-i)^\alpha(m-i+3+3\alpha) \end{bmatrix}, \quad (3.33)$$

and

$$\int_{t_i}^{t_{i+1}} (s - t_{i-2})(s - t_{i-1})(t_{m+1} - s)^{\alpha-1} ds = \begin{bmatrix} (m-i+1)^\alpha \begin{bmatrix} 2(m-i)^2 + (3\alpha+10)(m-i) \\ +2\alpha^2 + 9\alpha + 12 \end{bmatrix} \\ -(m-i)^\alpha \begin{bmatrix} 2(m-i)^2 + (5\alpha+10)(m-i) \\ +6\alpha^2 + 18\alpha + 12 \end{bmatrix} \end{bmatrix} \times \frac{(\Delta t)^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}. \quad (3.34)$$

Substituting these calculations into (3.31) produces the improved Atangana-Seda scheme predictor

$$\begin{aligned}
 y_{m+1}^P &= y_0 + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} \sum_{i=0}^1 f(t_i, y_i) [(m-i+1)^\alpha - (m-i)^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \sum_{i=0}^1 (f(t_{i+1}, y_{i+1}) - f(t_i, y_i)) \\
 &\times [(m-i+1)^{\alpha+1} - (m-i)^{\alpha+1} - (\alpha+1)(m-i)^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} \sum_{i=2}^m f(t_{i-2}, y_{i-2}) [(m-i+1)^\alpha - (m-i)^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \sum_{i=2}^m (f(t_{i-1}, y_{i-1}) - f(t_{i-2}, y_{i-2})) \\
 &\times \begin{bmatrix} (m-i+1)^\alpha(m-i+3+2\alpha) \\ -(m-i)^\alpha(m-i+3+3\alpha) \end{bmatrix} \\
 &+ \frac{(\Delta t)^\alpha}{2\Gamma(\alpha+3)} \sum_{i=2}^m [f(t_i, y_i) - 2f(t_{i-1}, y_{i-1}) + f(t_{i-2}, y_{i-2})] \\
 &\times \begin{bmatrix} (m-i+1)^\alpha \begin{bmatrix} 2(m-i)^2 + (3\alpha+10)(m-i) \\ +2\alpha^2 + 9\alpha + 12 \end{bmatrix} \\ -(m-i)^\alpha \begin{bmatrix} 2(m-i)^2 + (5\alpha+10)(m-i) \\ +6\alpha^2 + 18\alpha + 12 \end{bmatrix} \end{bmatrix}. \tag{3.35}
 \end{aligned}$$

In each iteration, the predictor (3.35) is calculated and then corrected by means of the implicit formula

$$\begin{aligned}
 y_{m+1} &= y_0 + Y_{m-1} + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} f(t_0, y_0) [(m+1)^\alpha - m^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} (f(t_1, y_1) - f(t_0, y_0)) [(m+1)^{\alpha+1} - m^{\alpha+1} - (\alpha+1)m^\alpha] \\
 &+ \frac{(\Delta t)^\alpha}{\Gamma(\alpha+1)} f(t_{m+1}, y_{m+1}^P) + \frac{\alpha(\Delta t)^\alpha}{\Gamma(\alpha+2)} (f(t_m, y_m) - f(t_{m+1}, y_{m+1}^P)) \\
 &- \frac{\alpha(\Delta t)^\alpha}{2\Gamma(\alpha+3)} (f(t_{m+1}, y_{m+1}^P) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})). \tag{3.36}
 \end{aligned}$$

3.1.1.3 Error Analysis

In this sub-section, we would like to present a detailed error analysis for the proposed Newton interpolation based predictor-corrector applied to the Caputo fractional differential equation (3.11).

Lemma 3.1.1. Subject to $f(., y(.)) \in C^3([0, T])$,

$$\mathcal{J}_1 := \left| \frac{1}{\Gamma(\alpha)} \sum_{i=0}^m \int_{t_i}^{t_{i+1}} (f(s, y(s)) - \mathcal{N}_i^P(s)) (t_{m+1} - s)^{\alpha-1} ds \right| \leq C \Delta t^p, \quad (3.37)$$

where $C > 0$ and

$$p = \begin{cases} 2 & \text{if } i \in \{0, 1\}, \\ 3 & \text{if } i \in \{2, \dots, m\}. \end{cases} \quad (3.38)$$

Proof. We have two distinct cases depending on the index i , namely $i \in \{0, 1\}$ and $i \in \{2, \dots, m\}$. We focus on the second case. The first case can be proven by following the same steps. According to the well-known Taylor's theorem, for $s \in [t_i, t_{i+1}]$, there exist $\Upsilon_i(s) \in [t_i, t_{i+1}]$ such that

$$\begin{aligned} \mathcal{J}_1 &\leq \frac{1}{\Gamma(\alpha)} \sum_{i=2}^m \int_{t_i}^{t_{i+1}} \left| \frac{f^{(3)}(\Upsilon_i(s), y(\Upsilon_i(s)))}{3!} (s - t_{i-2})(s - t_{i-1})(s - t_i) (t_{m+1} - s)^{\alpha-1} \right| ds \\ &\leq \frac{\mathcal{M}}{6\Gamma(\alpha)} \sum_{i=2}^m |(\bar{s}_i - t_{i-2})(\bar{s}_i - t_{i-1})(\bar{s}_i - t_i)| \int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds \\ &\leq \frac{\mathcal{M} \Delta t^3}{6\Gamma(\alpha)} \sum_{i=2}^m \int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds \\ &= \frac{\mathcal{M} \Delta t^3}{6\Gamma(\alpha+1)} \sum_{i=2}^m ((t_{m+1} - t_i)^\alpha - (t_{m+1} - t_{i+1})^\alpha) \\ &= \frac{\mathcal{M} t_{m-1}^\alpha}{6\Gamma(\alpha+1)} \Delta t^3, \end{aligned}$$

where $\mathcal{M} = \sup_{\delta \in [0, T]} |f^{(3)}(\delta, y(\delta))|$ and $\bar{s}_i \in [t_i, t_{i+1}]$ ■

Lemma 3.1.2. Subject to $f(., y(.)) \in C^3([0, T])$,

$$\left| \frac{1}{\Gamma(\alpha)} \sum_{i=0}^m \int_{t_i}^{t_{i+1}} (f(s, y(s)) - \mathcal{N}_i(s)) (t_{m+1} - s)^{\alpha-1} ds \right| \leq \tilde{C} \Delta t^q, \quad (3.39)$$

where $\tilde{C} > 0$ and

$$q = \begin{cases} 2 & \text{if } i = 0, \\ 3 & \text{if } i \in \{1, \dots, m\}. \end{cases} \quad (3.40)$$

Proof. This proof is analogous to that of Lemma 3.1.1 and thus has been omitted. ■

Theorem 3.1.1. Suppose that $f(\cdot, y(\cdot)) \in C^3([0, T])$ fulfils a Lipschitz condition with respect to its second variable. Then, for the predictor-corrector scheme (3.35-3.36), we have

$$\max_{0 \leq i \leq m+1} |y(t_i) - y_i| = \mathcal{O}(\Delta t^2). \quad (3.41)$$

Proof. Using the assumptions stated in the theorem, formulas (3.35) and (3.36), Lemmas 3.1.1 and 3.1.2, and simple mathematical induction for $0 \leq i \leq m + 1$, the result follows directly. ■

3.1.1.4 Caputo-Fabrizio fractional derivative

In this section, we will follow the same steps to derive a predictor-corrector scheme for the Caputo-Fabrizio fractional initial-value problem

$$\begin{cases} {}_0^{\text{CF}}D_t^\alpha y(t) = f(t, y(t)), \\ y(0) = y_0, \end{cases} \quad (3.42)$$

where the fractional order $\alpha \in (0, 1)$ and f is a nonlinear smooth function chosen such that system (3.42) admits a unique solution $y(t)$. Similar to the previous section, we apply the left-sided Caputo-Fabrizio fractional integral to both sides of the Caputo-Fabrizio fractional differential equation in (3.42) and incorporate the initial condition (cf. [80]) to produce

$$y(t) - y(0) = \frac{1 - \alpha}{M(\alpha)} f(t, y(t)) + \frac{\alpha}{M(\alpha)} \int_0^t f(s, y(s)) ds,$$

which when evaluated at two points in time $t_m = m\Delta t$ and $t_{m+1} = (m + 1)\Delta t$ yields

$$y(t_m) - y(0) = \frac{1 - \alpha}{M(\alpha)} f(t_m, y(t_m)) + \frac{\alpha}{M(\alpha)} \int_0^{t_m} f(s, y(s)) ds,$$

and

$$y(t_{m+1}) - y(0) = \frac{1-\alpha}{M(\alpha)} f(t_{m+1}, y(t_{m+1})) + \frac{\alpha}{M(\alpha)} \int_0^{t_{m+1}} f(s, y(s)) ds, \quad (3.43)$$

respectively. Taking the difference of the two points produces

$$y(t_{m+1}) - y(t_m) = \frac{1-\alpha}{M(\alpha)} [f(t_{m+1}, y(t_{m+1})) - f(t_m, y(t_m))] + \frac{\alpha}{M(\alpha)} \int_{t_m}^{t_{m+1}} f(s, y(s)) ds. \quad (3.44)$$

Function $f(s, y(s))$ can be approximated over the sub-interval $[t_m, t_{m+1}]$ by means of the same second order Newton polynomial (3.4), which was employed in the classical derivative case. The result is

$$\begin{aligned} y_{m+1} = & y_m + \frac{\alpha \Delta t}{M(\alpha)} f(t_{m+1}, y_{m+1}) + \frac{1-\alpha}{M(\alpha)} [f(t_{m+1}, y(t_{m+1})) - f(t_m, y(t_m))] \\ & + \frac{\alpha}{M(\alpha)} \left(\frac{f(t_{m+1}, y_{m+1}) - f(t_m, y_m)}{\Delta t} \right) \int_{t_m}^{t_{m+1}} (s - t_{m+1}) ds \\ & + \frac{\alpha}{M(\alpha)} \left(\frac{f(t_{m+1}, y_{m+1}) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})}{2(\Delta t)^2} \right) \\ & \times \int_{t_m}^{t_{m+1}} (s - t_m)(s - t_{m+1}) ds. \end{aligned} \quad (3.45)$$

Replacing the integrals by their respective values from (3.6) and (3.7) leads to the formula

$$\begin{aligned} y_{m+1} = & y_m + \frac{1-\alpha}{M(\alpha)} [f(t_{m+1}, y(t_{m+1})) - f(t_m, y(t_m))] \\ & + \frac{\alpha \Delta t}{M(\alpha)} f(t_{m+1}, y_{m+1}) - [f(t_{m+1}, y_{m+1}) - f(t_m, y_m)] \frac{\alpha \Delta t}{2M(\alpha)} \\ & - [f(t_{m+1}, y_{m+1}) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})] \frac{\alpha \Delta t}{12M(\alpha)}. \end{aligned} \quad (3.46)$$

Again, the terms y_{m+1} appearing on the right hand side of the implicit formula (3.46) are replaced by the prediction y_{m+1}^P obtained using the Atangana-Seda scheme developed for the Caputo-Fabrizio fractional derivative in [8]. This yields the implicit corrector formula

$$\begin{aligned} y_{m+1} = & y_m + \frac{1-\alpha}{M(\alpha)} [f(t_{m+1}, y_{m+1}^P) - f(t_m, y_m)] \\ & + \frac{\alpha}{M(\alpha)} \\ & \times \left[\frac{5}{12} f(t_{m+1}, y_{m+1}^P) \Delta t + \frac{2}{3} f(t_m, y_m) \Delta t - f(t_{m-1}, y_{m-1}) \frac{\Delta t}{12} \right], \end{aligned} \quad (3.47)$$

with the predictor term takes the following form:

$$\begin{aligned}
 y_{m+1}^p &= y_m + \frac{1-\alpha}{M(\alpha)} [f(t_m, y_m) - f(t_{m-1}, y_{m-1})] \\
 &\quad + \frac{\alpha}{M(\alpha)} \\
 &\quad \times \left[\frac{5}{12} f(t_{m-2}, y_{m-2}) \Delta t - \frac{4}{3} f(t_{m-1}, y_{m-1}) \Delta t + \frac{23}{12} f(t_m, y_m) \Delta t \right]. \quad (3.48)
 \end{aligned}$$

3.1.1.5 Atangana-Baleanu Fractional Derivative

The third type of fractional derivative we would like to consider is the Atangana-Baleanu derivative. Let us consider the initial-value problem

$$\begin{cases} {}_0^{\text{ABC}}D_t^\alpha y(t) = f(t, y(t)), \\ y(0) = y_0, \end{cases} \quad (3.49)$$

where, as usual, the fractional order $\alpha \in (0, 1)$ and f is a smooth nonlinear function that guarantees the existence of a unique solution $y(t)$ for (3.49). In order to obtain a predictor-corrector numerical scheme that solves (3.49), we apply the left-sided Atangana-Baleanu fractional integral to both sides of the Atangana-Baleanu fractional differential equation in (3.49) and incorporate the initial condition (cf. [9]) to produce

$$y(t) - y(0) = \frac{1-\alpha}{\text{AB}(\alpha)} f(t, y(t)) + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \int_0^t f(s, y(s))(t-s)^{\alpha-1} ds,$$

which leads to the approximation of $y(t)$ at $t_{m+1} = (m+1)\Delta t$ given by

$$y(t_{m+1}) = y(0) + \frac{1-\alpha}{\text{AB}(\alpha)} f(t_{m+1}, y(t_{m+1})) + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \sum_{i=0}^m \int_{t_i}^{t_{i+1}} f(s, y(s))(t_{m+1}-s)^{\alpha-1} ds, \quad (3.50)$$

where $t_0 = 0$. Using the Newton polynomial (3.14) to approximate function $f(s, y(s))$ in (3.50) yields

$$\begin{aligned}
 y(t_{m+1}) = & y(0) + \frac{1-\alpha}{\text{AB}(\alpha)} f(t_{m+1}, y(t_{m+1})) \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \int_0^{t_1} \left[f(t_0, y(t_0)) + \left(\frac{f(t_1, y(t_1)) - f(t_0, y(t_0))}{\Delta t} \right) s \right] (t_{m+1} - s)^{\alpha-1} ds \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \\
 & \times \sum_{i=1}^m \int_{t_i}^{t_{i+1}} \left\{ \begin{array}{l} f(t_{i+1}, y(t_{i+1})) \\ + \frac{f(t_{i+1}, y(t_{i+1})) - f(t_i, y(t_i))}{\Delta t} (s - t_{i+1}) \\ + \frac{f(t_{i+1}, y(t_{i+1})) - 2f(t_i, y(t_i)) + f(t_{i-1}, y(t_{i-1}))}{2(\Delta t)^2} \\ \times (s - t_i)(s - t_{i+1}) \end{array} \right\} (t_{m+1} - s)^{\alpha-1} ds, \quad (3.51)
 \end{aligned}$$

which can be simplified and rearranged to the form

$$\begin{aligned}
 y_{m+1} = & y_0 + \frac{1-\alpha}{\text{AB}(\alpha)} f(t_{m+1}, y(t_{m+1})) \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} f(t_0, y_0) \int_0^{t_1} (t_{m+1} - s)^{\alpha-1} ds \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \left(\frac{f(t_1, y_1) - f(t_0, y_0)}{\Delta t} \right) \int_0^{t_1} s (t_{m+1} - s)^{\alpha-1} ds \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \sum_{i=1}^m f(t_{i+1}, y_{i+1}) \int_{t_i}^{t_{i+1}} (t_{m+1} - s)^{\alpha-1} ds \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \sum_{i=1}^m \frac{f(t_{i+1}, y_{i+1}) - f(t_i, y_i)}{\Delta t} \int_{t_i}^{t_{i+1}} (s - t_{i+1}) (t_{m+1} - s)^{\alpha-1} ds \\
 & + \frac{\alpha}{\text{AB}(\alpha)\Gamma(\alpha)} \sum_{i=1}^m \frac{f(t_{i+1}, y_{i+1}) - 2f(t_i, y_i) + f(t_{i-1}, y_{i-1})}{2(\Delta t)^2} \\
 & \times \int_{t_i}^{t_{i+1}} (s - t_i)(s - t_{i+1}) (t_{m+1} - s)^{\alpha-1} ds. \quad (3.52)
 \end{aligned}$$

Replacing the integrals with their respective values from (3.19)-(3.22) leads to

$$\begin{aligned}
 y_{m+1} = & y_0 + \frac{1-\alpha}{\text{AB}(\alpha)} f(t_{m+1}, y(t_{m+1})) \\
 & + \frac{\alpha(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+1)} f(t_0, y_0) [(m+1)^\alpha - m^\alpha] \\
 & + \frac{\alpha(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+2)} (f(t_1, y_1) - f(t_0, y_0)) [(m+1)^{\alpha+1} - m^{\alpha+1} - (\alpha+1)m^\alpha] \\
 & + \frac{\alpha(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+1)} \sum_{i=1}^m f(t_{i+1}, y_{i+1}) [(m-i+1)^\alpha - (m-i)^\alpha] \\
 & + \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \sum_{i=1}^m (f(t_{i+1}, y_{i+1}) - f(t_i, y_i)) [(m-i-\alpha)(m-i+1)^\alpha - (m-i)^{\alpha+1}] \\
 & + \frac{(\Delta t)^\alpha}{2\Gamma(\alpha+3)} \sum_{i=1}^m (f(t_{i+1}, y_{i+1}) - 2f(t_i, y_i) + f(t_{i-1}, y_{i-1})) \\
 & \times \begin{bmatrix} (m-i+1)^\alpha [2(m-i)^2 - \alpha(m-i+1) + 2(m-i)] \\ -(m-i)^\alpha [2(m-i)^2 + \alpha(m-i) + 2(m-i)] \end{bmatrix}. \tag{3.53}
 \end{aligned}$$

Using the notation Y_{m-1} defined earlier in (3.24)-(3.25) and replacing the terms y_{m+1} on the right hand side of the formula by the predicted value y_{m+1}^P , we obtain the predictor-corrector method described by the implicit formula

$$\begin{aligned}
 y_{m+1} = & y_0 + \frac{1-\alpha}{\text{AB}(\alpha)} f(t_{m+1}, y_{m+1}^P) + \frac{\alpha}{\text{AB}(\alpha)} Y_{m-1} + \frac{\alpha(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+1)} f(t_0, y_0) [(m+1)^\alpha - m^\alpha] \\
 & + \frac{\alpha(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+2)} (f(t_1, y_1) - f(t_0, y_0)) [(m+1)^{\alpha+1} - m^{\alpha+1} - (\alpha+1)m^\alpha] \\
 & + \frac{\alpha(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+1)} f(t_{m+1}, y_{m+1}^P) + \frac{\alpha^2(\Delta t)^\alpha}{\text{AB}(\alpha)\Gamma(\alpha+2)} (f(t_m, y_m) - f(t_{m+1}, y_{m+1}^P)) \\
 & - \frac{\alpha^2(\Delta t)^\alpha}{2\text{AB}(\alpha)\Gamma(\alpha+3)} (f(t_{m+1}, y_{m+1}^P) - 2f(t_m, y_m) + f(t_{m-1}, y_{m-1})), \tag{3.54}
 \end{aligned}$$

with the improved explicit Atangana-Seda predictor

$$\begin{aligned}
 y_{m+1}^P &= y_0 + \frac{1-\alpha}{AB(\alpha)} f(t_m, y_m) + \frac{\alpha(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha+1)} \sum_{i=0}^1 f(t_i, y_i) [(m-i+1)^\alpha - (m-i)^\alpha] \\
 &+ \frac{\alpha(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha+2)} \sum_{i=0}^1 (f(t_{i+1}, y_{i+1}) - f(t_i, y_i)) \\
 &\times [(m-i+1)^{\alpha+1} - (m-i)^{\alpha+1} - (\alpha+1)(m-i)^\alpha] \\
 &+ \frac{\alpha(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha+1)} \sum_{i=2}^m f(t_{i-2}, y_{i-2}) [(m-i+1)^\alpha - (m-i)^\alpha] \\
 &+ \frac{\alpha(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha+2)} \sum_{i=2}^m (f(t_{i-1}, y_{i-1}) - f(t_{i-2}, y_{i-2})) \\
 &\times \begin{bmatrix} (m-i+1)^\alpha(m-i+3+2\alpha) \\ -(m-i)^\alpha(m-i+3+3\alpha) \end{bmatrix} \\
 &+ \frac{\alpha(\Delta t)^\alpha}{2AB(\alpha)\Gamma(\alpha+3)} \sum_{i=2}^m [f(t_i, y_i) - 2f(t_{i-1}, y_{i-1}) + f(t_{i-2}, y_{i-2})] \\
 &\times \begin{bmatrix} (m-i+1)^\alpha [2(m-i)^2 + (3\alpha+10)(m-i) + 2\alpha^2 + 9\alpha + 12] \\ -(m-i)^\alpha [2(m-i)^2 + (5\alpha+10)(m-i) + 6\alpha^2 + 18\alpha + 12] \end{bmatrix}. \quad (3.55)
 \end{aligned}$$

Note that this predictor is obtained in the same way as that of the Caputo derivative in Section 3.1.1.2.

Concluding Remarks

Remark 3.1.1.

- The predictor term y_{m+1}^P used in each of the previous scenarios can be replaced by any other scheme including, for instance, the ones in [27, 77]. In the cases of the Caputo-Fabrizio/Atangana-Baleanu fractional derivatives, some minor modifications would have to be made to the methods.
- In the initial-value problem (3.11), if $n-1 < \alpha \leq n \in \mathbb{N}$ and $y_0 = (y_{0,1}, \dots, y_{0,n})$, then the initial value y_0 on the right hand side of (3.35) and (3.36) needs to be replaced by the sum

$$\sum_{k=0}^{n-1} \frac{t_{m+1}^k}{k!} y_{0,k+1}.$$

3.1.2 Examples and numerical experiments

In this section, we will present simulation results obtained by means of the predictor-corrector numerical methods proposed in this paper for different initial value problems. In the last example, we will consider a fractional activator-inhibitor Gierer-Meinhardt model whose dynamics are to be analyzed based on the obtained numerical solutions. Throughout this section, we use the absolute error

$$\max_{0 \leq i \leq m+1} |y(t_i) - y_i|.$$

In addition, we use the acronyms: predictor-corrector (PC), proposed predictor-corrector (PPC), Atangana-Seda (AS), improved Atangana-Seda (IAS), two step Adams-Moulton (TSAM), and three step Adams-Bashforth (TSAB).

Example 3.1.1. We start with the classical initial-value problem

$$\begin{cases} \frac{dy(t)}{dt} = 2y(t) + 3, \\ y(0) = 1, \end{cases} \quad (3.56)$$

which has the exact solution

$$y(t) = \frac{5}{2}e^{2t} - \frac{3}{2}. \quad (3.57)$$

Figure 3.1 depicts the exact solution (3.57) along with the numerical solutions obtained by means of the proposed method and the standard Atangana-Seda method. The absolute error results are shown in Table 3.1 for different values of the numerical step size. We see that the proposed method for the classical derivative given in (3.9) as well as the Caputo method in (3.36) applied with $\alpha = 1$ achieve a considerably lower error than the two-step Adams-Bashforth (cf. [14, p. 110]) methods.

Example 3.1.2. Let us consider another initial-value problem with a classical derivative:

$$\begin{cases} \frac{dy(t)}{dt} = -\cos(2t)y^2(t), \\ y(0) = 1. \end{cases} \quad (3.58)$$

The exact solution of this problem is known to be

$$y(t) = \frac{2}{2 + \sin(2t)}. \quad (3.59)$$

The exact solution (3.59) is depicted in Figure 3.2 alongside the numerical solution obtained by means of the proposed numerical scheme (3.9) and the Atangana-Seda solution. The error performance is detailed in Table 3.2. Again, the proposed schemes achieve a noticeably superior performance.

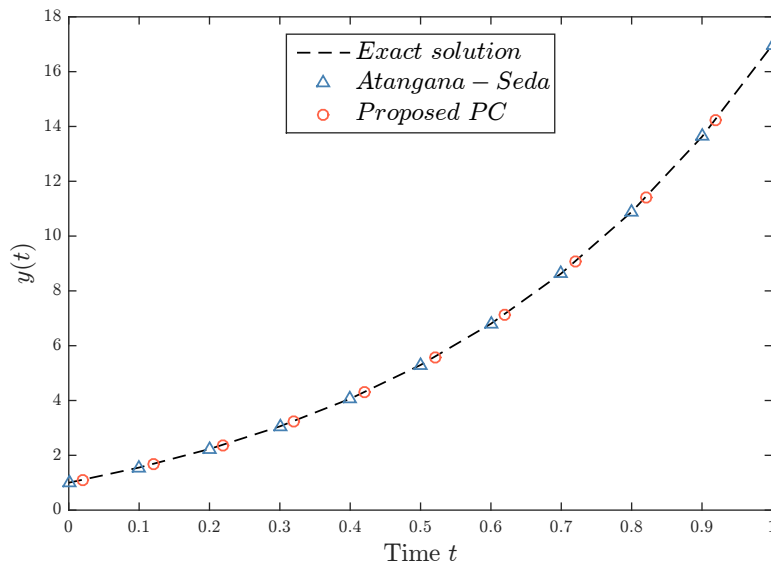


Figure 3.1: Solution of problem (3.56) for $t \in [0, 1]$.

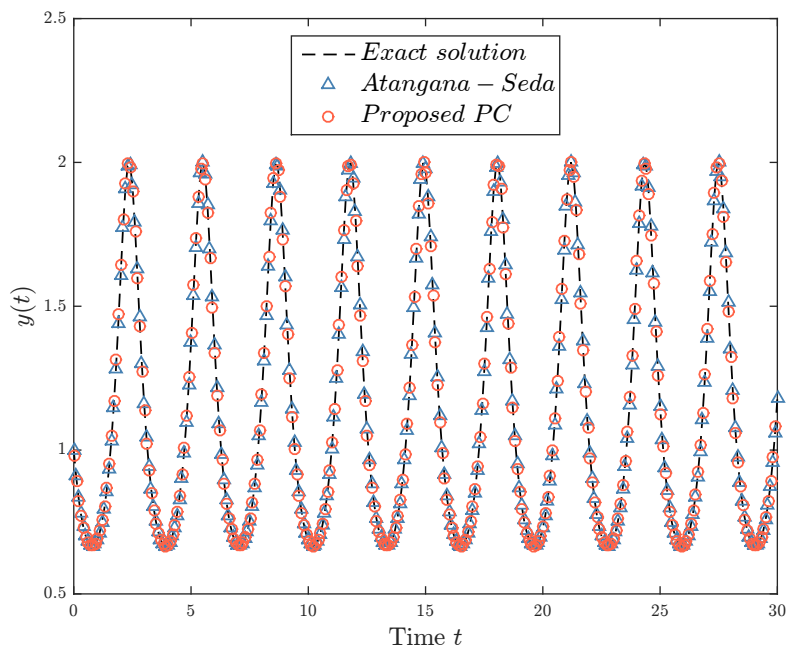


Figure 3.2: Solution of problem (3.58) for $t \in [0, 30]$.

Table 3.1: Comparison of the absolute error of various numerical methods for problem (3.56) with $t \in [0, 1]$.

Method	$\Delta t = \frac{1}{16}$	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{200}$	$\Delta t = \frac{1}{1024}$
Proposed PC (3.36) fractional, $\alpha = 1$	2.6019×10^{-3}	7.8442×10^{-5}	2.9104×10^{-6}	2.2690×10^{-8}
Proposed PC (3.9)	4.7391×10^{-3}	9.6052×10^{-5}	3.3246×10^{-6}	2.5281×10^{-8}
Atangana-Seda [8]	2.0657×10^{-2}	3.9611×10^{-4}	1.3570×10^{-5}	1.0281×10^{-7}
Two-step Adams-Bashforth	2.0503×10^{-1}	1.4503×10^{-2}	1.5223×10^{-3}	5.8597×10^{-5}

Table 3.2: Comparison of the absolute error of various numerical methods for problem (3.58) with $t \in [0, 30]$.

Method	$\Delta t = \frac{1}{16}$	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{200}$	$\Delta t = \frac{1}{700}$
Proposed PC (3.36) fractional, $\alpha = 1$	8.3152×10^{-3}	2.2772×10^{-5}	6.5114×10^{-7}	2.6151×10^{-8}
Proposed PC (3.9)	8.9834×10^{-3}	1.0474×10^{-4}	3.1725×10^{-6}	7.1930×10^{-8}
Atangana-Seda [8]	2.2712×10^{-2}	3.4369×10^{-4}	1.1236×10^{-5}	2.6193×10^{-7}
Two-step Adams-Bashforth	2.1387×10^{-2}	1.3589×10^{-3}	1.3984×10^{-4}	1.1436×10^{-5}

Example 3.1.3. Next, we consider the fractional Caputo initial-value problem

$$\begin{cases} {}_0^C D_t^\alpha y(t) = t^\beta, \\ y(0) = 0, \end{cases} \quad (3.60)$$

for some real constant β , which admits the unique exact solution

$$y(t) = \frac{\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 1)} t^{\alpha + \beta}. \quad (3.61)$$

Figure 3.3 shows the exact solution (3.61) along with the numerical solution obtained by means of the proposed predictor corrector scheme (3.36) and the standard and improved Atangana-Seda methods for $\beta = 0.9$ and $\alpha \in \{0.25, 0.87\}$. The absolute error results are presented in Table 3.3 for the same value of β and $\alpha \in \{0.25, 0.56, 0.87\}$ with different numerical step sizes. In all scenarios, the absolute error achieved by the proposed method is lower than the improved Atangana-Seda method, which in turn is lower than the standard one.

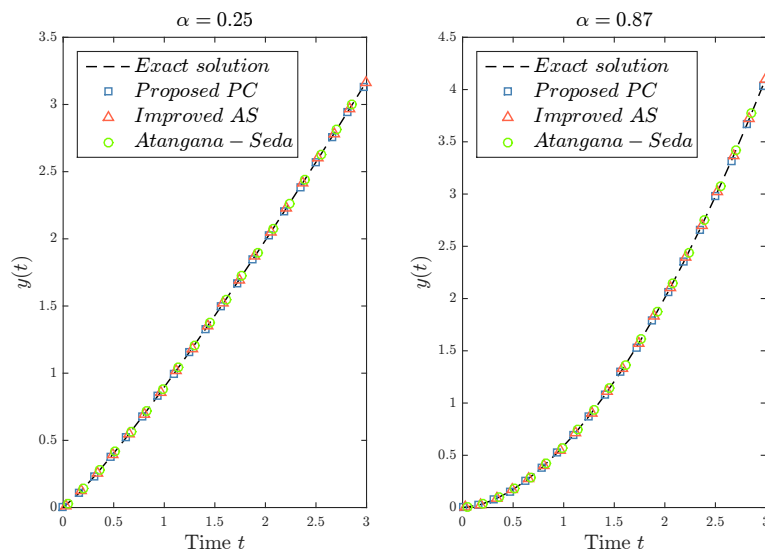


Figure 3.3: Solution of problem (3.60) for $\beta = 0.9$ and $t \in [0, 3]$.

Table 3.3: Comparison of the absolute error of various methods for problem (3.60) with $\beta = 0.9$ and $t \in [0, 3]$.

Method	$\alpha = 0.25$			$\alpha = 0.56$			$\alpha = 0.87$		
	$\Delta t = \frac{1}{100}$	$\Delta t = \frac{1}{800}$	$\Delta t = \frac{1}{100}$	$\Delta t = \frac{1}{100}$	$\Delta t = \frac{1}{400}$	$\Delta t = \frac{1}{100}$	$\Delta t = \frac{1}{100}$	$\Delta t = \frac{1}{200}$	
PPC (3.36)	6.8792×10^{-5}	6.2948×10^{-6}	2.8000×10^{-5}	3.6996×10^{-6}	7.6132×10^{-6}	4.4095×10^{-7}			
IAS (3.35)	3.9492×10^{-4}	3.6137×10^{-5}	8.4439×10^{-5}	1.1157×10^{-5}	1.9429×10^{-5}	1.1253×10^{-6}			
AS [8]	2.3016×10^{-3}	2.1060×10^{-4}	1.2783×10^{-3}	1.6891×10^{-4}	4.9855×10^{-4}	2.8876×10^{-5}			

Example 3.1.4. Let us consider the fractional Caputo initial-value problem

$$\begin{cases} {}_0^C D_t^\alpha y(t) = \frac{2t^{2-\alpha}}{\Gamma(3-\alpha)} - \frac{t^{1-\alpha}}{\Gamma(2-\alpha)} - y(t) - t + t^2, \\ y(0) = 0. \end{cases} \quad (3.62)$$

The exact solution of (3.62) can be shown to be

$$y(t) = t^2 - t. \quad (3.63)$$

Figure 3.4 and Table 3.4 present the numerical solutions of (3.62) in comparison to the exact solution (3.63) for different fractional orders and numerical steps sizes. Again, the proposed method (3.36) is superior to the Atangana-Seda method and the improved method (3.35).

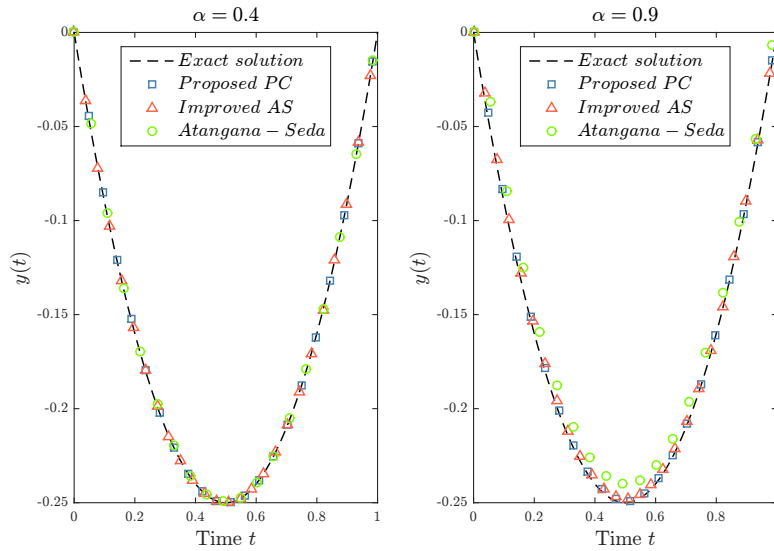


Figure 3.4: Solution of problem (3.62) for $t \in [0, 1]$.

Table 3.4: Comparison of the absolute error of various methods for problem (3.62) with $t \in [0, 1]$.

Method	$\alpha = 0.4$			$\alpha = 0.65$			$\alpha = 0.9$		
	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{512}$	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{512}$	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{64}$	$\Delta t = \frac{1}{512}$	$\Delta t = \frac{1}{512}$
PPC (3.36)	7.6806×10^{-4}	6.4455×10^{-5}	3.1549×10^{-3}	3.1549×10^{-3}	4.5513×10^{-4}	6.4490×10^{-3}	6.4490×10^{-3}	8.2593×10^{-4}	8.2593×10^{-4}
IAS (3.35)	5.7442×10^{-3}	7.0486×10^{-4}	8.8970×10^{-3}	8.8970×10^{-3}	1.1129×10^{-3}	1.2365×10^{-2}	1.2365×10^{-2}	1.5685×10^{-3}	1.5685×10^{-3}
AS [8]	1.5787×10^{-2}	2.0038×10^{-3}	2.5879×10^{-2}	2.5879×10^{-2}	3.2837×10^{-3}	3.4087×10^{-2}	3.4087×10^{-2}	4.3577×10^{-3}	4.3577×10^{-3}

Example 3.1.5. In the previous examples, we considered some simple single differential equations with known exact solutions. Let us now analyze a realistic fractional activator-inhibitor model using analytical stability theory and validate the theoretical results numerically by means of the proposed method. Consider the system described by

$$\begin{cases} {}_0^C D_t^\alpha a(t) = \varrho_0 \varrho + c \varrho \frac{a(t)^2}{h(t)} - \mu a(t), \\ {}_0^C D_t^\alpha h(t) = c' \varrho' a(t)^2 - \nu h(t), \\ a(0) = a_0, \quad h(0) = h_0, \end{cases} \quad (3.64)$$

where $a(t)$ and $h(t)$ denote the concentrations of the activator and inhibitor substances at time instant t , respectively. The constants $\varrho_0, \varrho, c, \mu, c', \varrho', a_0, h_0$ and ν are assumed to be positive real numbers, and the fractional differentiation order $\alpha \in (0, 1]$. For $\alpha = 1$, system (3.64) reduces to the well known Gierer-Meinhardt model describing the morphogenesis process [43, 93]. Morphogenesis is the biological process driving living organisms to take specific shapes. Inclusion of a diffusion part in the Gierer-Meinhardt model was useful in modeling the head formation of a fresh-water animal known as hydra [42]. It is well established that system (3.64) admits the unique equilibrium point (cf. [93]):

$$E^* = (a^*, h^*), \quad (3.65)$$

where

$$a^* = \frac{\varrho_0 \varrho c' \varrho' + c \varrho \nu}{\mu c' \varrho'}, \quad (3.66)$$

and

$$h^* = \frac{c' \varrho'}{\nu} (a^*)^2. \quad (3.67)$$

Evaluating the Jacobian matrix of system (3.64) at the unique equilibrium E^* yields

$$J|_{E^*} = \begin{pmatrix} \frac{2c\mu\nu}{c\nu+c'\varrho'\varrho_0} - \mu & -\frac{c}{\varrho} \left(\frac{\mu\nu}{c\nu+c'\varrho'\varrho_0} \right)^2 \\ \frac{2\varrho(c\nu+c'\varrho'\varrho_0)}{\mu} & -\nu \end{pmatrix}. \quad (3.68)$$

The determinant and trace of the Jacobian are given by

$$\text{tr}J|_{E^*} = \frac{2\mu\nu c}{\nu c + \varrho_0 \varrho' c'} - \mu - \nu, \quad (3.69)$$

and

$$\det J|_{E^*} = \mu\nu, \quad (3.70)$$

respectively. Hence, the characteristic equation of associated with E^* is

$$\lambda^2 - \lambda \operatorname{tr}J|_{E^*} + \det J|_{E^*} = 0, \quad (3.71)$$

leading to the eigenvalues

$$\lambda_{1,2} = \frac{1}{2} \left(\operatorname{tr}J|_{E^*} \pm \sqrt{\operatorname{tr}^2J|_{E^*} - 4\det J|_{E^*}} \right). \quad (3.72)$$

The dynamics of (3.64) can be analyzed by means of the results in [5, Section 3]. Firstly, if the discriminant of (3.71) is equal to zero, i.e.

$$\operatorname{tr}^2J|_{E^*} - 4\det J|_{E^*} = 0, \quad (3.73)$$

the eigenvalues (3.72) reduce to the real quantity

$$\lambda_{1,2} = \frac{1}{2} \operatorname{tr}J|_{E^*}. \quad (3.74)$$

Hence, the equilibrium E^* is asymptotically stable when $\operatorname{tr}J|_{E^*} < 0$ and unstable when $\operatorname{tr}J|_{E^*} > 0$ for all $\alpha \in (0, 1]$.

Secondly, if the discriminant is strictly positive, i.e.

$$\operatorname{tr}^2J|_{E^*} - 4\det J|_{E^*} > 0, \quad (3.75)$$

the eigenvalues (3.72) are also real. However, we distinguish two cases with respect to the asymptotic stability:

- If $\operatorname{tr}J|_{E^*} > 0$, then

$$\lambda_1 = \frac{1}{2} \left(\operatorname{tr}J|_{E^*} + \sqrt{\operatorname{tr}^2J|_{E^*} - 4\det J|_{E^*}} \right) > 0. \quad (3.76)$$

Thus, $|\arg(\lambda_1)| = 0$ and E^* is unstable for all $\alpha \in (0, 1]$.

- If $\operatorname{tr}J|_{E^*} < 0$, then

$$|\arg(\lambda_{1,2})| = \pi > \frac{\alpha\pi}{2} \text{ for } \alpha \in (0, 1]. \quad (3.77)$$

Thus, E^* is asymptotically stable for all $\alpha \in (0, 1]$.

Thirdly, if the discriminant is strictly negative, i.e.

$$\operatorname{tr}^2J|_{E^*} - 4\det J|_{E^*} < 0, \quad (3.78)$$

the eigenvalues become

$$\lambda_{1,2} = \frac{1}{2} \left(\operatorname{tr}J|_{E^*} \pm i \sqrt{4\det J|_{E^*} - \operatorname{tr}^2J|_{E^*}} \right), \quad (3.79)$$

leading to three distinguishable cases:

- If $\text{tr}J|_{E^*} = 0$, then

$$\lambda_{1,2} = \pm i\sqrt{\det J|_{E^*}}, \quad (3.80)$$

leading to

$$|\arg(\lambda_{1,2})| = \frac{\pi}{2} > \frac{\alpha\pi}{2} \text{ for } \alpha \in (0, 1). \quad (3.81)$$

Hence, E^* is asymptotically stable for all $\alpha \in (0, 1)$.

- If $\text{tr}J|_{E^*} < 0$, then

$$|\arg(\lambda_{1,2})| > \frac{\pi}{2} > \frac{\alpha\pi}{2} \text{ for } \alpha \in (0, 1), \quad (3.82)$$

and, consequently, E^* is asymptotically stable for all $\alpha \in (0, 1]$.

- If $\text{tr}J|_{E^*} > 0$, then E^* is asymptotically stable for all $\alpha \in (0, 1)$ if

$$\tan^2(|\arg(\lambda_{1,2})|) = \frac{4\mu\nu(cv + \varrho_0\varrho'c')^2}{(c\nu(\mu - \nu) - \varrho_0\varrho'c'(\mu + \nu))^2} > \tan^2\left(\frac{\alpha\pi}{2}\right) + 1, \quad (3.83)$$

and unstable for all $\alpha \in (0, 1)$ if

$$\frac{4\mu\nu(cv + \varrho_0\varrho'c')^2}{(c\nu(\mu - \nu) - \varrho_0\varrho'c'(\mu + \nu))^2} < \tan^2\left(\frac{\alpha\pi}{2}\right) + 1. \quad (3.84)$$

Remark 3.1.2. If the unique equilibrium E^* of (3.64) is unstable for some $\alpha \in (0, 1)$, then E^* is also unstable for $\alpha = 1$. Since an exact solution is not available for system (3.64), visualizing the system dynamics requires numerical solutions, which can be obtained using the proposed predictor-corrector method described by (3.35)-(3.36). The parameters adopted for the simulations are listed in Table 3.5.

Table 3.5: Parameter values of system (3.64) adopted in the numerical simulations.

Parameter	ϱ_0	ϱ	μ	ν	c	ϱ'	c'	a_0	h_0
Value	1	1	4	2	3	1	1	2	3

Condition (3.78) can be easily verified and $\text{tr}J|_{E^*} = \frac{6}{7} > 0$. For $\alpha = 0.85$, we have

$$\tan^2(|\arg(\lambda_{1,2})|) = \frac{392}{9} > \tan^2\left(\frac{\alpha\pi}{2}\right) + 1 \approx 18.3497, \quad (3.85)$$

which implies that the equilibrium $E^* = (\frac{7}{4}, \frac{49}{32})$ is asymptotically stable. The numerical solutions and corresponding phase plot depicted in Figures 3.5 and 3.6, respectively, agree with the theoretical analysis as the solution converges towards $(\frac{7}{4}, \frac{49}{32})$. For $\alpha = 0.95$, we have

$$\tan^2(|\arg(\lambda_{1,2})|) = \frac{392}{9} < \tan^2\left(\frac{\alpha\pi}{2}\right) + 1 \approx 162.4476, \quad (3.86)$$

and thus, the equilibrium $E^* = (\frac{7}{4}, \frac{49}{32})$ is unstable. Again, the numerical results shown in in Figures 3.7 and 3.8 coincide with the theoretical results as the solution is periodically stable around $(\frac{7}{4}, \frac{49}{32})$. According to Remark 2, we conclude that the equilibrium E^* of (3.64) is unstable for $\alpha = 1$. This result is confirmed by the numerical results depicted in Figures 3.9 and 3.10.

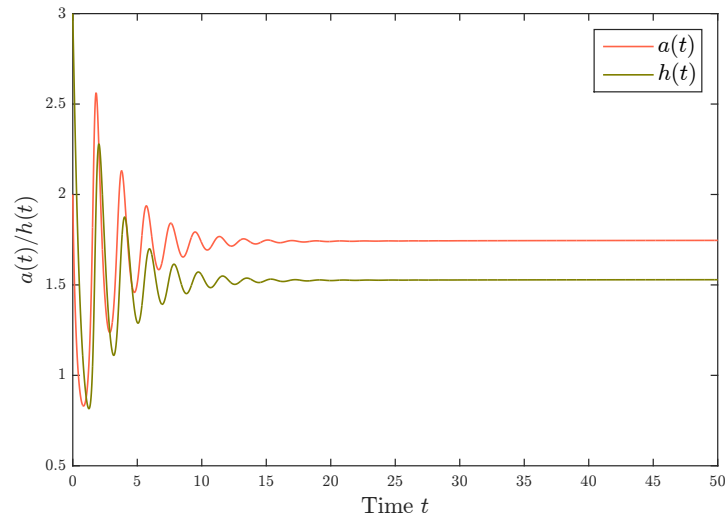


Figure 3.5: The numerical solution of system (3.64) for $\alpha = 0.85$ with the parameters listed in Table 3.5.

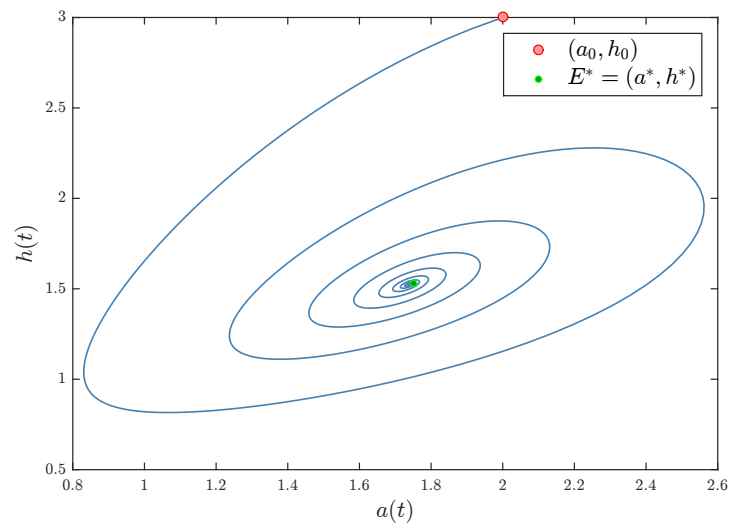


Figure 3.6: Phase plot of system (3.64) for $\alpha = 0.85$ with the parameters listed in Table 3.5.

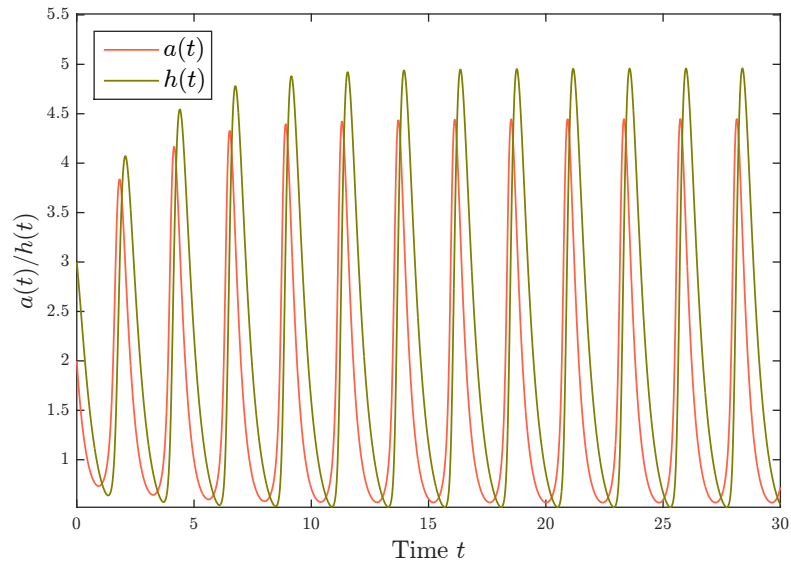


Figure 3.7: The numerical solution of system (3.64) for $\alpha = 0.95$ with the parameters listed in Table 3.5.

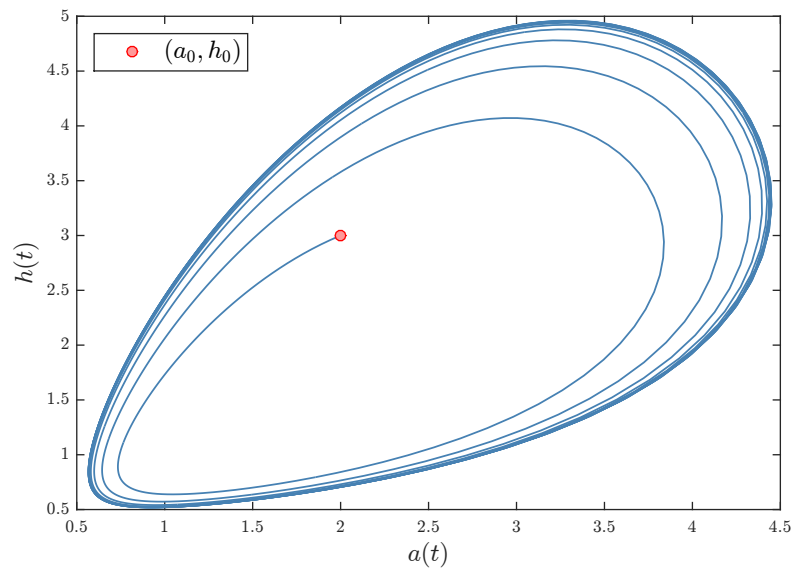


Figure 3.8: Phase plot of system (3.64) for $\alpha = 0.95$ with the parameters listed in Table 3.5.

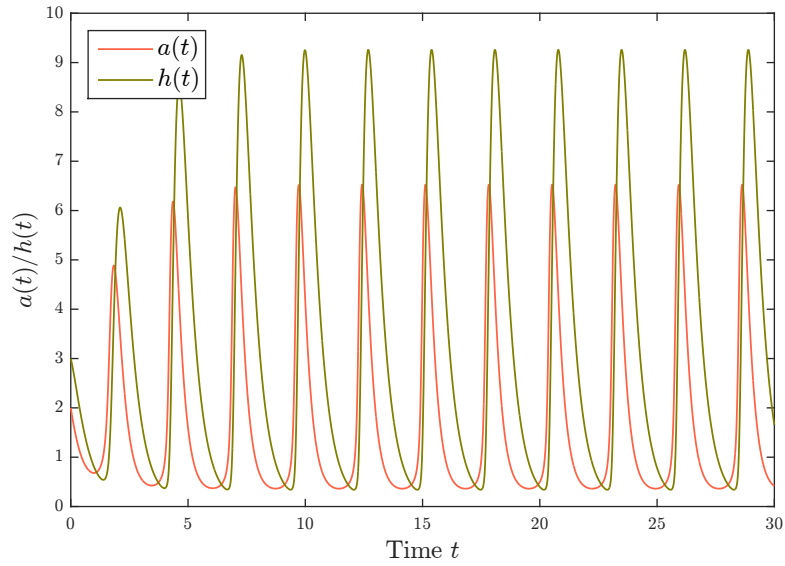


Figure 3.9: The numerical solution of system (3.64) for $\alpha = 1$ with the parameters listed in Table 3.5.

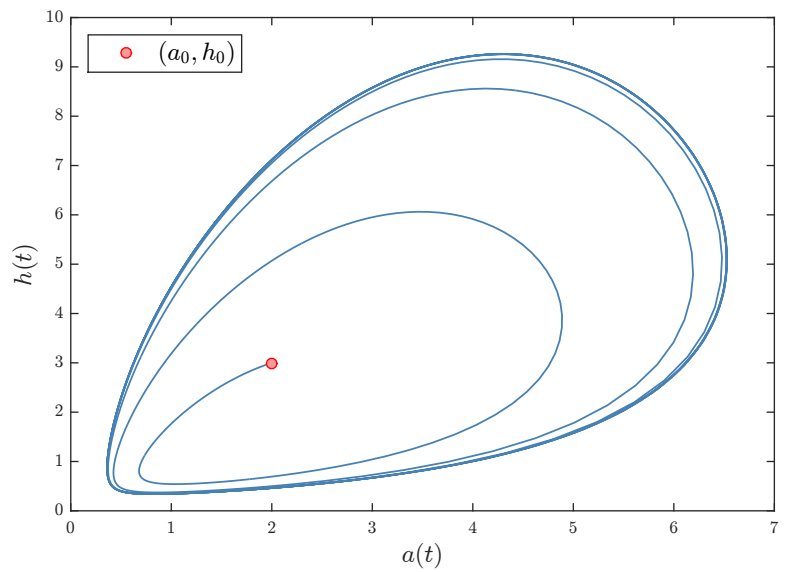


Figure 3.10: Phase plot of system (3.64) for $\alpha = 1$ with the parameters listed in Table 3.5.

3.2 A predictor-corrector method for variable-order fractional delay-differential systems with multiple lags

Due to its effectiveness in real world fractional delay differential equations is receiving importance in various branches of science [25, 38, 54], the last one is dynamical systems involving non-integer order as well as time delays. The delay introduces information from the past and introduction it in the model enriches its dynamics and allows a precise description of the real life phenomena, the applications of delay differential equations is clearly observed in many practical systems such as neuroscience, automatic control, traffic models, lasers, and so on [24, 36].

On the other hand, a fractional calculus has been acknowledged as a promising mathematical tool to efficiently describe the historical memory and hereditary properties of complex dynamic systems [40]. However, various literature indicated that the memory and hereditary properties of the system may change with time or other conditions [63, 102]. Hence, the variable-order fractional derivatives provide an excellent approach for the modeling of memory and hereditary properties [98, 100].

The variable-order fractional calculus are an extension of the classical fractional calculus, namely the order of fractional derivatives or integrals depends on the time and/or another variable. In 1993, Samko and Ross [95] firstly proposed the variable-order integral and differential as well as some basic properties. After that, the variable-order differential operators have been discussed by several authors [20, 96, 101]. Since the kernel of the variable order derivatives which appear in differential equations has a variable-exponent, analytical solutions of variable order fractional differential equations are more difficult to obtain, thus the effective and applicable numerical techniques for solving such equations are always needed. But numerical techniques to solve variable order fractional differential equations are at the early stage of growth. Several recent researches concerned with the existence, uniqueness and numerical solutions of variable order fractional delay differential equations [103, 71, 50].

The purpose of this section is to present numerical solutions of variable-order fractional delay differential equations with multiple lags based on the Adams-Bashforth-Moulton method, where the derivative is defined in the Caputo variable-order fractional sense. Since the variable-order fractional derivatives contain classical and fractional derivatives as special cases and also single delay is a special case of multiple delays, several results of references are significantly generalized. The error analysis for this method is given and the effectiveness of the algorithm is highlighted with numerical examples.

3.2.1 Formulation of numerical method

Throughout this sub-section we denote by VOFDDEs for variable-order fractional delay-differential equations with multiple lags.

In this part, we modified the Adams-Bashforth-Moulton predictor-corrector method described in [28] to solve VOFDDEs. We consider VOFDDEs defined by

$${}_0^C D_t^{\alpha(t)} y(t) = \Psi(t, y(t), y(t - \tau_1), \dots, y(t - \tau_k)), \quad t \in [0, T], \quad k \in \mathbb{N}^*, \quad (3.87)$$

$$y(t) = \phi(t), \quad t \in [-\tau, 0], \quad \tau = \max\{\tau_1, \dots, \tau_k\}, \quad (3.88)$$

where $y(t) = (y_1, \dots, y_N)$, $N \in \mathbb{N}^*$, $T > 0$, $0 < \alpha(t) \leq 1$ and $\tau_j \geq 0$, $j = 1, \dots, k$; denotes the delay coefficients. Furthermore, we assume that $\Psi \in C([0, T] \times \mathbb{R}^{kN+N}, \mathbb{R}^N)$. Consider a uniform grid $\left\{ t_i = ih : i = -m_j, -m_j + 1, \dots, -1, 0, 1, \dots, n \right\}$, where m_j and n are integers such that $n = \lceil \frac{T}{h} \rceil$ and $m_j = \lceil \frac{\tau_j}{h} \rceil$, for $j = 1, \dots, k$. Note that

$$y(t_i - \tau_j) = y(ih - m_j h) = y(t_{i-m_j}), \quad i = 0, \dots, n; \quad j = 1, \dots, k. \quad (3.89)$$

Now, the approximation to the delayed term $y(t_i - \tau_j)$ which consist of the following two types.

- **When τ_j is constant.** Suppose that $(m_j - \delta_j)h = \tau_j$ with $0 \leq \delta_j < 1$. When $\delta_j = 0$, $y(t_i - \tau_j)$ can be approximated by

$$y(t_i - \tau_j) \approx \begin{cases} y_{i-m_j} & \text{if } i > m_j \\ \phi_i & \text{if } i \leq m_j \end{cases}, \quad j = 1, \dots, k. \quad (3.90)$$

When $0 < \delta_j < 1$, $j = 1, \dots, k$ cannot be calculated directly. Let $\omega_{i+1, j}$ be the approximation to $y(t_{i+1} - \tau_j)$ for the case $(m_j - 1)h < \tau_j < m_j h$, $j = 1, \dots, k$. On interpolating it by the two nearest points, that is

$$\omega_{i+1, j} = \delta_j y_{i-m_j+2} + (1 - \delta_j) y_{i-m_j+1}, \quad (3.91)$$

the last equality implies the implicit of the numerical equation if $m_j > 1$ which can be directly determined. However, when $m_j = 1$ and $\delta_j \neq 0$, that is $\tau_j < h$ the first term in the right-hand side of (3.91) is $\delta_j y_{i+1}$. Further prediction is required in this case, that is

$$\omega_{i+1, j} = \delta_j y_{i+1}^P + (1 - \delta_j) y_i. \quad (3.92)$$

- **When τ_j is time varying.** If $\tau_j = \tau_j(t)$ the approximation seems to be intricate.

Let

$\omega_{i+1,j} \approx y(t_{i+1} - \tau_j)$, the linear interpolation of y_l at point $t = t_{i+1} - \tau_j(t_{i+1})$ is used to approximate the delay term. Let $\tau_j(t_{i+1}) = (m_{i+1,j} - \delta_{i+1,j})h$ where $m_{i+1,j} \in \mathbb{Z}_+$ and $\delta_{i+1,j} \in [0, 1)$, then

$$\omega_{i+1,j} = \delta_{i+1,j} y_{i-m_{i+1,j}+2} + (1 - \delta_{i+1,j}) y_{i-m_{i+1,j}+1}. \quad (3.93)$$

Further prediction is required if $m_{i+1,j} = 1$ in the first term in the right-hand side of (3.93) and it is not needed if $m_{i+1,j} > 1$. Hence in each step of the computational procedure, a condition $m_{i,j} = 1$ or not is initially checked for further prediction or not.

Without loss of generality, we restrict to the first case study, we display the numerical algorithm for VOFDDEs (3.87)-(3.88).

By applying ${}_0I_{t_{i+1}}^{\alpha(t_{i+1})}$ on both sides of (3.87) and using (3.88), we get to:

$$y(t_{i+1}) = \phi(0) + \frac{1}{\Gamma(\alpha(t_{i+1}))} \int_0^{t_{i+1}} (t_{i+1} - \sigma)^{\alpha(t_{i+1}-1)} \Psi(\sigma, y(\sigma - \tau_1), \dots, y(\sigma - \tau_k)) d\sigma. \quad (3.94)$$

Further, the integral in equation (3.94) is evaluated using product trapezoidal quadrature formula. Then by using (3.89) the corrector formula is thus (we denote the numerical calculation of y by \bar{y})

$$\begin{aligned} \bar{y}(t_{i+1}) = & \phi(0) + \frac{h^{\alpha_{i+1}}}{\Gamma(\alpha_{i+1} + 2)} \Psi(t_{i+1}, \bar{y}(t_{i+1}), \bar{y}(t_{i+1}-m_1), \dots, \bar{y}(t_{i+1}-m_k)) \\ & + \frac{h^{\alpha_{i+1}}}{\Gamma(\alpha_{i+1} + 2)} \sum_{j=0}^i a_{j,i+1} \Psi(t_j, \bar{y}(t_j), \bar{y}(t_j-m_1), \dots, \bar{y}(t_j-m_k)), \end{aligned} \quad (3.95)$$

where $\alpha_{i+1} = \alpha(t_{i+1})$ and

$$a_{j,i+1} = \begin{cases} i^{\alpha_{i+1}+1} - (i - \alpha_{i+1})(i+1)^{\alpha_{i+1}}, & j = 0, \\ (i-j+2)^{\alpha_{i+1}+1} - 2(i-j+1)^{\alpha_{i+1}+1} + (i-j)^{\alpha_{i+1}+1}, & 1 \leq j \leq i-1, \\ 2(2^{\alpha_{i+1}} - 1), & j = i, \\ 1, & j = i+1. \end{cases} \quad (3.96)$$

Now, we replace $\bar{y}(t_{i+1})$ on the right hand side of (3.95) by an approximation $\bar{y}^P(t_{i+1})$, called predictor. Product rectangle rule is used in (3.94) to derive predictor term:

$$\bar{y}^P(t_{i+1}) = \phi(0) + \frac{h^{\alpha_{i+1}}}{\Gamma(\alpha_{i+1} + 1)} \sum_{j=0}^i b_{j,i+1} \Psi(t_j, \bar{y}(t_j), \bar{y}(t_j-m_1), \dots, \bar{y}(t_j-m_k)), \quad (3.97)$$

where

$$b_{j,i+1} = \begin{cases} (i-j+1)^{\alpha_{i+1}} - (i-j)^{\alpha_{i+1}}, & 0 \leq j \leq i-1, \\ 1, & j = i. \end{cases} \quad (3.98)$$

The algorithm to solve (3.87)-(3.88) is as follows

Algorithm 1 Solving fractional delay-differential system with multiple lags.

Input: $\Psi = [\Psi_1, \dots, \Psi_N], \alpha(t), \tau = [\tau_1, \dots, \tau_k], T, \phi(t) = [\phi_1(t), \dots, \phi_N(t)], h$.

1. Compute values $n, m_j, \delta_j, \alpha_i$.
2. Set, $M = \max\{m_1, \dots, m_k\}$.
3. For $i = 0 : -1 : -M$, $\bar{y}(ih) = \phi(ih)$.
4. For $i = 1 : n$ do
 - Compute $\bar{y}(t_i - \tau_j)$;
 - Compute $\bar{y}^P(t_{i+1})$;
 - Evaluate $\omega_{i+1,j}$;
 - Compute $\bar{y}(t_{i+1})$.

Output: $\phi(-Mh), \phi(-Mh+h), \dots, \phi(-h), \phi(0), \bar{y}(t_1), \dots, \bar{y}(t_n)$.

3.2.2 Error analysis of the numerical scheme

Under the following condition on Ψ ,

$$\|\Psi(t, u_1, u_2, \dots, u_{k+1}) - \Psi(t, w_1, w_2, \dots, w_{k+1})\|_{\mathbb{R}^N} \leq \sum_{j=1}^{k+1} L_j \|u_j - w_j\|_{\mathbb{R}^N}, \quad (3.99)$$

for all $t \in [0, T]$, $u_j, w_j \in \mathbb{R}^N$ and $L_j > 0$, for $j = 1, \dots, k+1$. we can get

Theorem 3.2.1. Suppose the solution $y \in C^2([0, T])$ of (3.87)-(3.88) satisfies the following two conditions:

$$\left\| \int_0^{t_{i+1}} (t_{i+1} - \sigma)^{\alpha_{i+1}-1} {}_0^C D_{\sigma}^{\alpha_{i+1}} y(\sigma) d\sigma - \frac{h^{\alpha_{i+1}}}{\alpha_{i+1}} \sum_{j=0}^i b_{j,i+1} {}_0^C D_t^{\alpha_{i+1}} y(t_j) \right\|_{\mathbb{R}^N} \leq C t_{i+1}^{\gamma_1} h^{\theta_1}, \quad (3.100)$$

$$\left\| \int_0^{t_{i+1}} (t_{i+1} - \sigma)^{\alpha_{i+1}-1} {}_0^C D_{\sigma}^{\alpha_{i+1}} y(\sigma) d\sigma - \frac{h^{\alpha_{i+1}}}{\alpha_{i+1}(\alpha_{i+1} + 1)} \sum_{j=0}^i a_{j,i+1} {}_0^C D_t^{\alpha_{i+1}} y(t_j) \right\|_{\mathbb{R}^N} \leq C t_{i+1}^{\gamma_2} h^{\theta_2}, \quad (3.101)$$

with some $\gamma_1, \gamma_2 \geq 0$, and $\theta_1, \theta_2 > 0$, then for some suitable $T > 0$, we have

$$\max_{0 \leq j \leq n} \|y(t_j) - \bar{y}(t_j)\|_{\mathbb{R}^N} \leq \mathcal{K} h^q, \quad (3.102)$$

where $n = \lceil \frac{T}{h} \rceil$, $q = \min\{\theta_1 + \alpha(t), \theta_2\}$, and C, \mathcal{K} are a positive constants.

Proof. We prove the result by using the mathematical induction. Suppose that the conclusion is true for $j = 0, \dots, i$. From the assumptions (3.99), note that

$$\|\Psi(t, u_1, u_2, \dots, u_{k+1}) - \Psi(t, w_1, w_2, \dots, w_{k+1})\|_{\mathbb{R}^N} \leq C_N h^q \sum_{j=1}^{k+1} L_j, \quad (3.103)$$

where $C_N > 0$, from (3.87), (3.103) and the following inequality

$$\frac{h^{\alpha_{i+1}}}{\alpha_{i+1}} \sum_{j=0}^i b_{j,i+1} \leq \frac{T^{\alpha_{i+1}}}{\alpha_{i+1}}, \quad (3.104)$$

we have

$$\|y(t_{i+1}) - \bar{y}^P(t_{i+1})\|_{\mathbb{R}^N} \leq \frac{CT^{\gamma_1}}{\Gamma(\alpha_{i+1})} h^{\theta_1} + \frac{C_1 T^{\alpha_{i+1}}}{\Gamma(\alpha_{i+1} + 1)} h^q, \quad (3.105)$$

where $C_1 > 0$. Since

$$\frac{h^{\alpha_{i+1}}}{\alpha_{i+1}(\alpha_{i+1} + 1)} \sum_{j=0}^i a_{j,i+1} \leq T^{\alpha_{i+1}} \quad (3.106)$$

and thanks to (3.101), (3.103), (3.105), we have

$$\|y(t_{i+1}) - \bar{y}(t_{i+1})\|_{\mathbb{R}^N} \leq \mathcal{K} h^q. \quad (3.107)$$

For the detailed, see [103].

3.2.3 Examples and numerical experiments

The computer code of Algorithm 1, was written in Matlab, and the time step used in the simulation was $h = \frac{1}{10}$.

Example 3.2.1. Consider a VOFDDEs version of delay differential equation given in [112]

$$\begin{cases} {}_0^C D_t^{\alpha(t)} y(t) = \frac{2y(t-2)}{1+y(t-2.6)^{9.65}} - y(t), \\ y(t) = 0.5, \quad t \leq 0. \end{cases} \quad (3.108)$$

The approximate solution of (3.108) for fractional derivative $\alpha = 0.95$ is shown in Fig. 3.11, whereas Fig. 3.12 shows phase portrait of the system i.e. plots of $y(t)$ versus $y(t-2)$

and $y(t)$ versus $y(t-2.6)$ for the same value of α . It be analysed from this figures that the system (3.108) shows chaotic behaviour almost different to those generated by a single delay (see [103]).

Fig. 3.13 shows the numerical solution of (3.108) for the variable order fractional derivative $\alpha(t) = 0.93 - \frac{1}{e^t+1}$, and phase portrait of the system (3.108) for $\alpha(t) = 0.93 - \frac{1}{e^t+1}$ is shown in Fig. 3.14. In the following experiment, we have changed the variable order fractional derivative by $\alpha(t) = \frac{2.8+\sin(t)}{4}$, and the approximate solution is shown in Fig. 3.15, Fig. 3.16 shows the phase portrait of the system (3.108) for the same value of derivative.

The portrait phase of the variable order fractional derivative (Fig. 3.14 and Fig. 3.16) shows us that the chaotic behaviour is more complicated than fractional derivative and thus the general behavior of the solution of system (3.108) depends on kind of derivative.

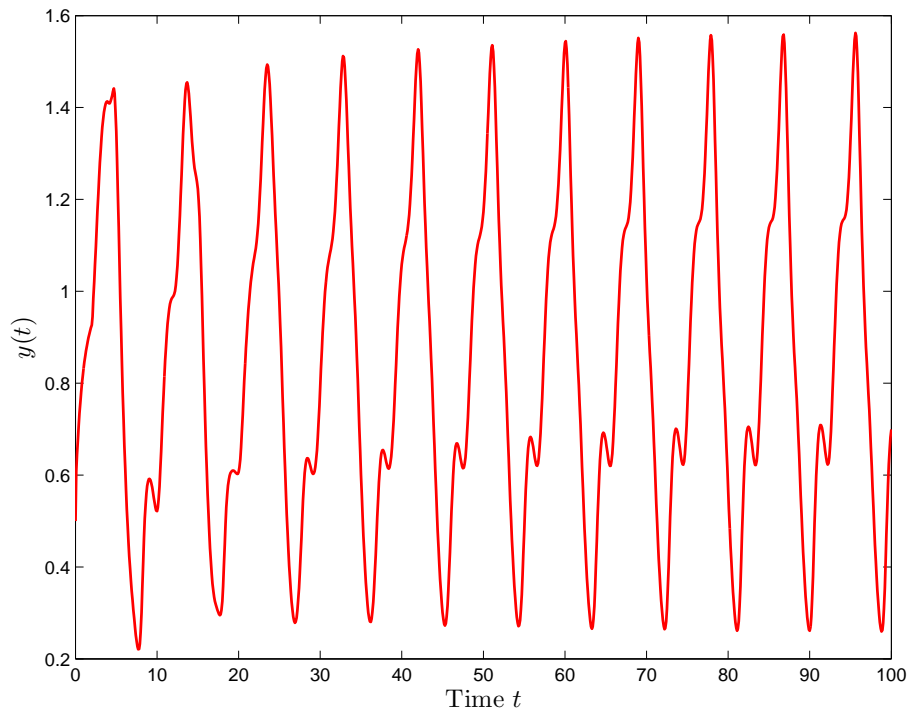


Figure 3.11: The numerical solution of system (3.108) with fractional derivative.

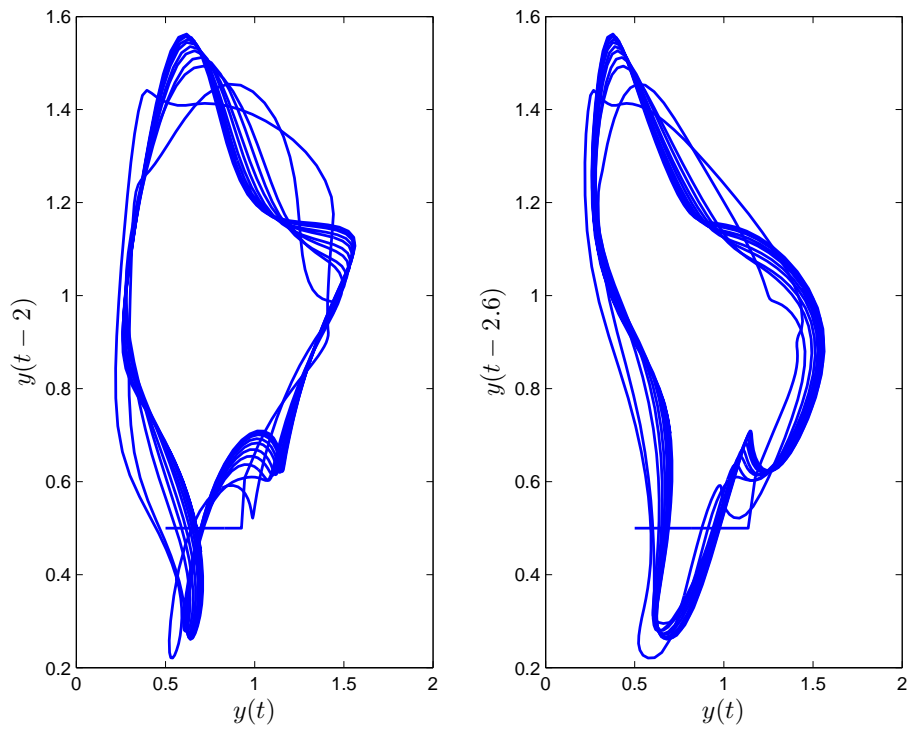


Figure 3.12: Phase plot of system (3.108) with fractional derivative.

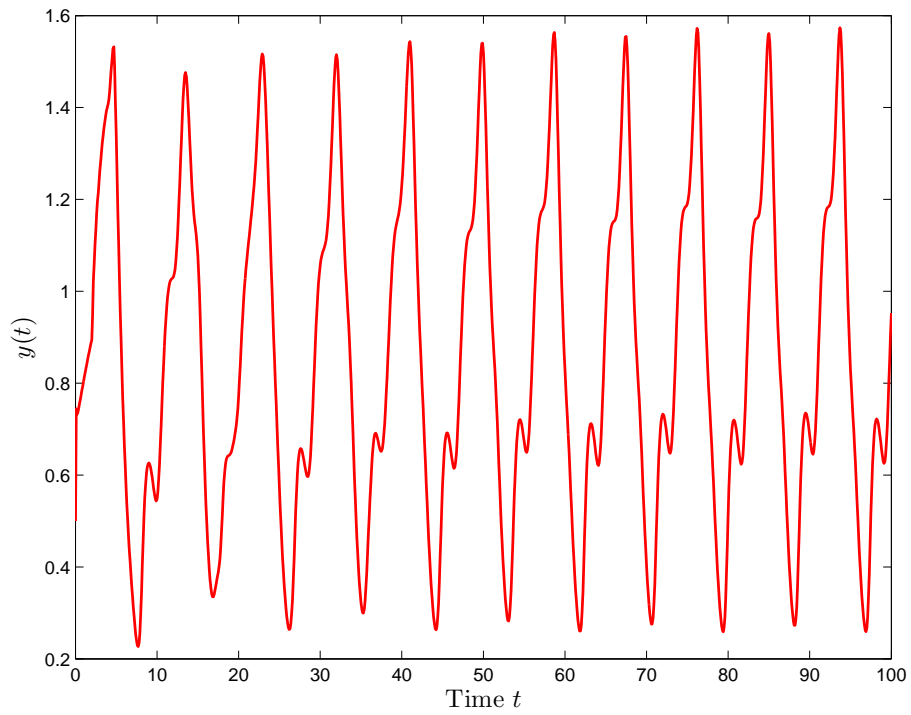


Figure 3.13: The numerical solution of system (3.108) with VO fractional derivative.

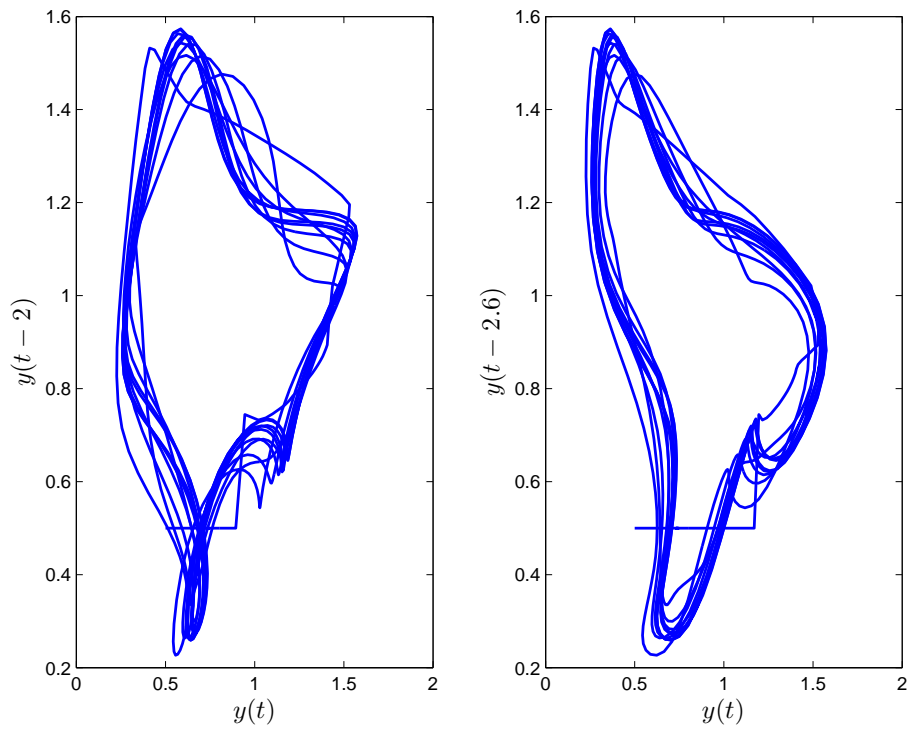


Figure 3.14: Phase plot of system (3.108) with VO fractional derivative.

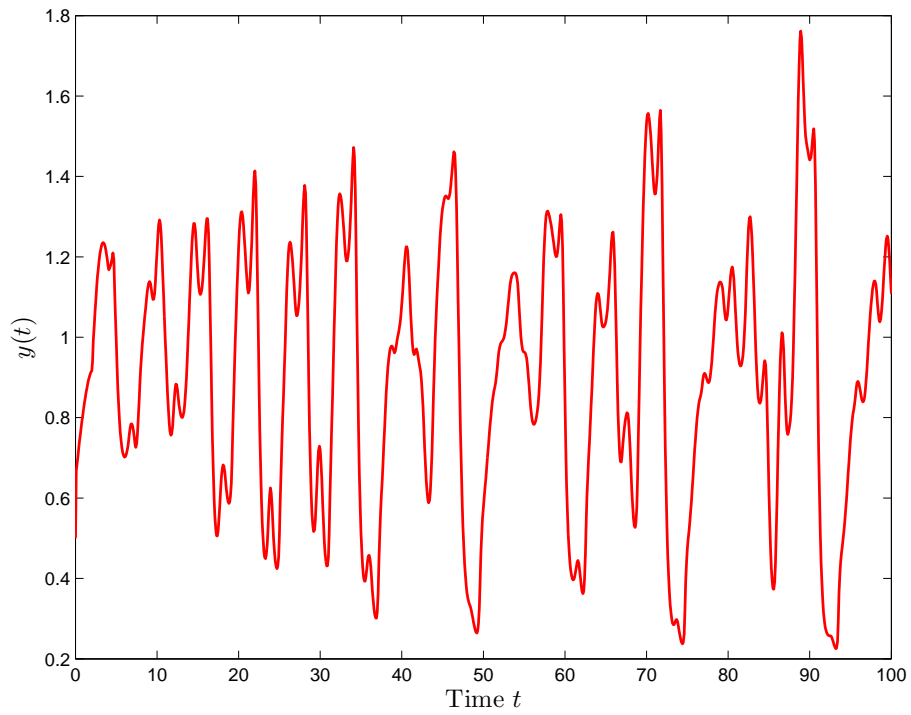


Figure 3.15: The numerical solution of system (3.108) with VO fractional derivative.

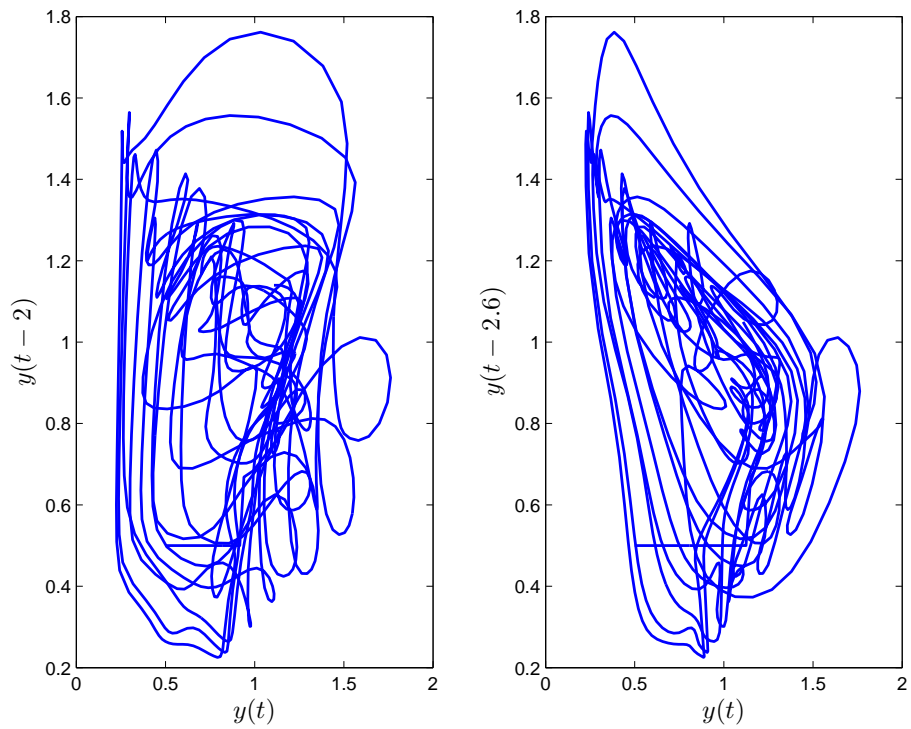


Figure 3.16: Phase plot of system (3.108) with VO fractional derivative.

Example 3.2.2. Consider a VOFDDEs version of four dimensional enzyme kinetics with an inhibitor molecule given in [78]

$$\begin{cases} {}_0^C D_t^{\alpha(t)} y_1(t) &= 10.5 - \frac{y_1(t)}{1+0.0005y_4^3(t-4)}, \\ {}_0^C D_t^{\alpha(t)} y_2(t) &= \frac{y_1(t)}{1+0.0005y_4^3(t-4.8)} - y_2(t), \\ {}_0^C D_t^{\alpha(t)} y_3(t) &= y_2(t) - y_3(t), \\ {}_0^C D_t^{\alpha(t)} y_4(t) &= y_3(t) - y_4(t), \\ y(t) &= [60, 10, 10, 20]^T, \quad t \leq 0. \end{cases} \quad (3.109)$$

where $y(t) = [y_1(t), y_2(t), y_3(t), y_4(t)]^T$.

The approximate solution of (3.109) for fractional derivative $\alpha(t) = 0.98$ is shown in Fig. 3.17, which looks a bit different to the system (3.109) generated by a single delay (see [103]). In Fig. 3.18, we depict approximate solutions of system (3.109) for variable order fractional derivative $\alpha(t) = 0.97 - \frac{1}{e^t+1}$, Fig. 3.19 shows numerical solution of system (3.109) for variable order fractional derivative $\alpha(t) = 0.93 - \frac{1}{e^t+1}$. In the following, we have selected the variable order fractional derivative $\alpha(t) = \frac{2.8+\sin(t)}{4}$, it has many variation on $[0, 160]$, Fig. 3.20, showed a completely different behavior of system (3.109).

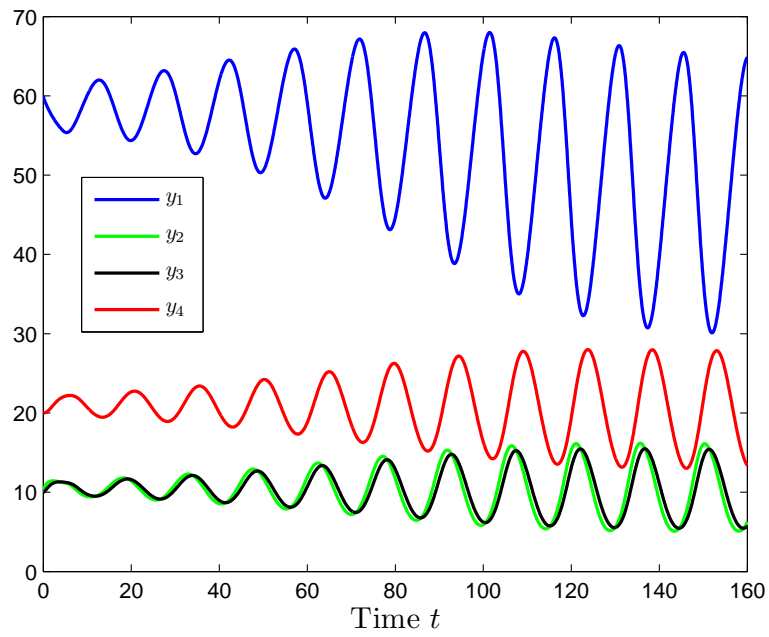


Figure 3.17: The numerical solution of system (3.109) with $\alpha(t) = 0.98$.

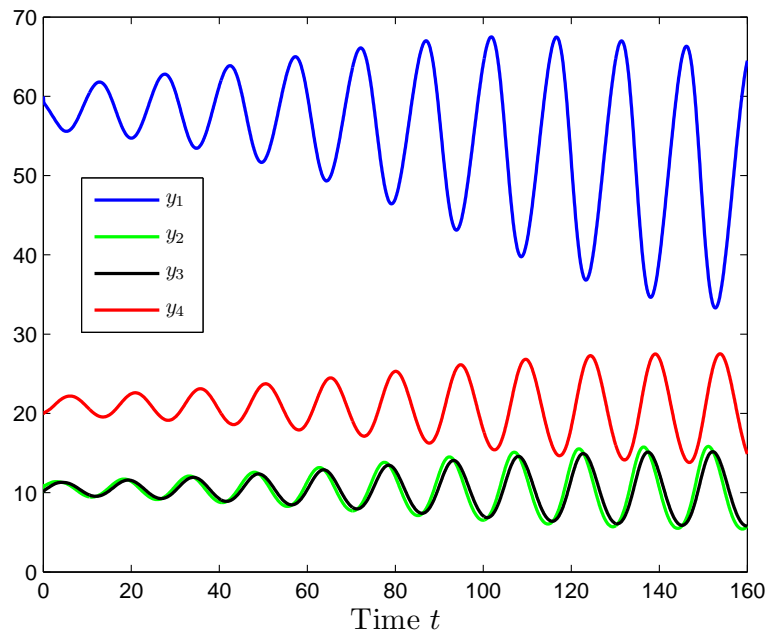


Figure 3.18: The numerical solution of system (3.109) with $\alpha(t) = 0.97 - \frac{1}{e^{t+1}}$.

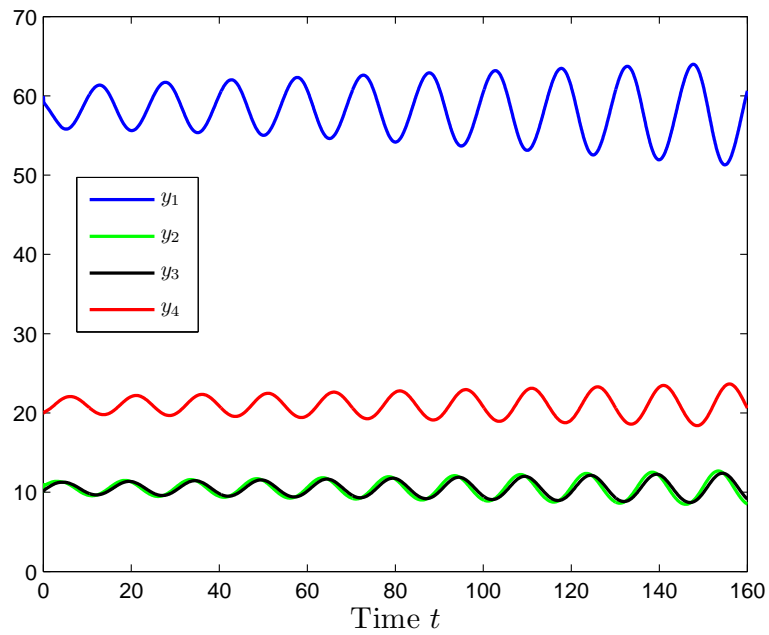


Figure 3.19: The numerical solution of system (3.109) with $\alpha(t) = 0.93 - \frac{1}{e^{t+1}}$.

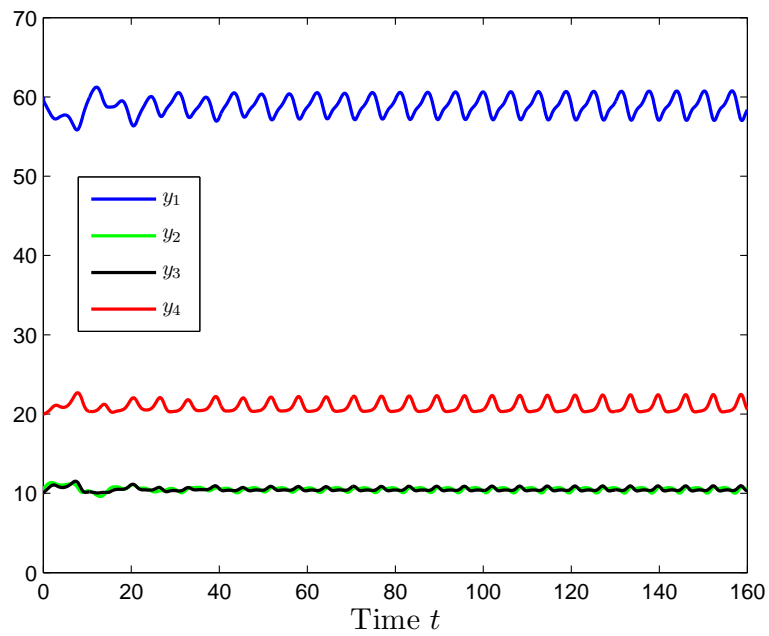


Figure 3.20: The numerical solution of system (3.109) with $\alpha(t) = \frac{2.8 + \sin(t)}{4}$.

3.3 Method of lines for time-fractional reaction-diffusion systems

In this section, We propose a numerical method for solving time fractional order reaction diffusion system. The numerical method are obtained considering the Method of Lines (MOL) approach, the partial derivatives with respect to the space variables are discretized to obtain a system of ODEs in the time and then the algorithms in previous two sections can be used to solve this fractional ODE system. This method is compared with the finite difference method applied to a specific model of time fractional order reaction-diffusion.

3.3.1 Numerical simulation of time-fractional reaction diffusion systems

We consider the following time-fractional reaction-diffusion system (TFRD):

$$\left\{ \begin{array}{l} {}^C D_{0,t}^{\alpha_1} u - d_1 \frac{\partial^2 u}{\partial x^2} = F(u, v) \quad \text{in } \Omega_T, \\ {}^C D_{0,t}^{\alpha_2} v - d_2 \frac{\partial^2 v}{\partial x^2} = G(u, v) \quad \text{in } \Omega_T, \\ u(x, 0) = \varphi(x) \quad \text{on } \Omega, \\ v(x, 0) = \psi(x) \quad \text{on } \Omega, \\ \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = 0, \quad \text{on } \partial\Omega. \end{array} \right. \quad (3.110)$$

Where $\Omega = [0, L]$, $\Omega_T = [0, L] \times [0, T]$, $\partial\Omega = \{0, L\}$; $d_1, d_2, L, T > 0$, $u := u(x, t)$, $v := v(x, t)$, $0 < \alpha_j \leq 1$ for $j = 1, 2$; We assume that the functions F, G, φ, ψ satisfy the conditions in order that the solution of the system (3.110) exists and is unique.

The first step in our solution process is to replace $\frac{\partial^2 u}{\partial x^2}$, $\frac{\partial^2 v}{\partial x^2}$ in the first and second equations of (3.110) by a finite difference approximation accurate to order such as

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}, \quad \frac{\partial^2 v_i}{\partial x^2} = \frac{v_{i-1} - 2v_i + v_{i+1}}{\Delta x^2}, \quad i = \overline{1, N}. \quad (3.111)$$

Where $\Delta x = \frac{L}{N}$, $N \in \mathbb{N} - \{1, 2\}$, and $u_i = u(i\Delta x, t)$, $v_i = v(i\Delta x, t)$. The region is divided into the strips by $N+1$ dividing straight lines (hence the name method of lines) parallel to the t direction, therefore system (3.110) becomes a system of fractional order differential equations and can be written in matrix form as

$$\begin{cases} {}^C D_{0,t}^{\alpha_1} U(t) = d_1 A U(t) + (F(u_0, v_0), \dots, F(u_N, v_N))^T & \text{in } [0, T], \\ {}^C D_{0,t}^{\alpha_2} V(t) = d_2 A V(t) + (G(u_0, v_0), \dots, G(u_N, v_N))^T & \text{in } [0, T], \\ U(0) = U_0, V(0) = V_0. \end{cases} \quad (3.112)$$

Where, A is an $(N + 1) \times (N + 1)$ matrix given by

$$A = \frac{1}{h^2} \begin{pmatrix} -2 & 2 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ 0 & 1 & -2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -2 & 1 & 0 \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \dots & 0 & 2 & -2 \end{pmatrix}, \quad (3.113)$$

and $U(t) = (u_0, \dots, u_N)^T$, $V(t) = (v_0, \dots, v_N)^T$, $U_0 = (\varphi(0), \varphi(\Delta x), \dots, \varphi(N\Delta x))^T$, $V_0 = (\psi(0), \psi(\Delta x), \dots, \psi(N\Delta x))^T$. Now, we can solve the system (3.112) by the suggested algorithms in the previous two sections.

3.3.1.1 Examples and numerical experiments

We consider specific time-fractional reaction-diffusion model, with the Schnackenberg nonlinear reaction (see [31]):

$$F(u(x, t), v(x, t)) = 0.14 - u(x, t) + u^2(x, t)v(x, t), \quad G(u(x, t), v(x, t)) = 0.54 - u^2(x, t)v(x, t).$$

The unique positive constant steady state solution is denoted by $E_* = (u_*, v_*)$, where

$$u_* = a + b, \quad v_* = \frac{b}{(a + b)^2}.$$

We choice different parameters for simulation, as the table below shown:

	Figures ($k = 1, 2$)	$\alpha_j, j = 1, 2$	d_1	d_2	L	T	$\varphi(x)$	$\psi(x)$
set 1	A_k, C_k	$\alpha_1 = \alpha_2 = \sqrt{\frac{5}{9}}$	0.01	0.02	8	50	$0.68 + \frac{\cos(x)}{10}$	$0.78 + \frac{\cos(x)}{10}$
set 2	B_k, D_k	$\alpha_1 = \frac{1}{3}, \alpha_2 = \frac{1}{2}$	0.01	0.02	8	120	$0.68 + \frac{\cos(x)}{12}$	$0.78 + \frac{\sin(x)}{12}$

The Numerical solutions are obtained by finite difference method (FDM) and method of lines (MOL).

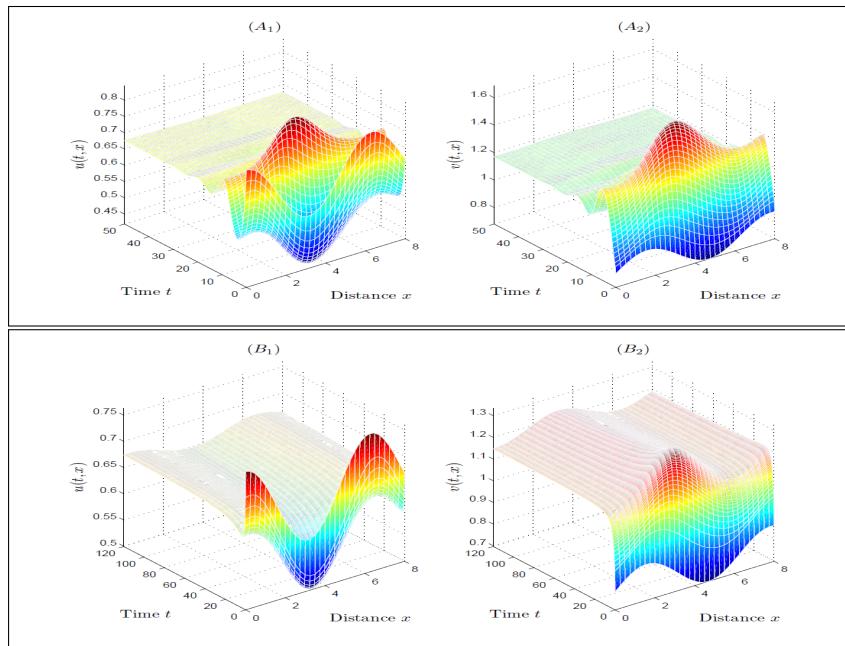


Figure 3.21: The numerical solution of time-fractional Schnackenberg model by FDM

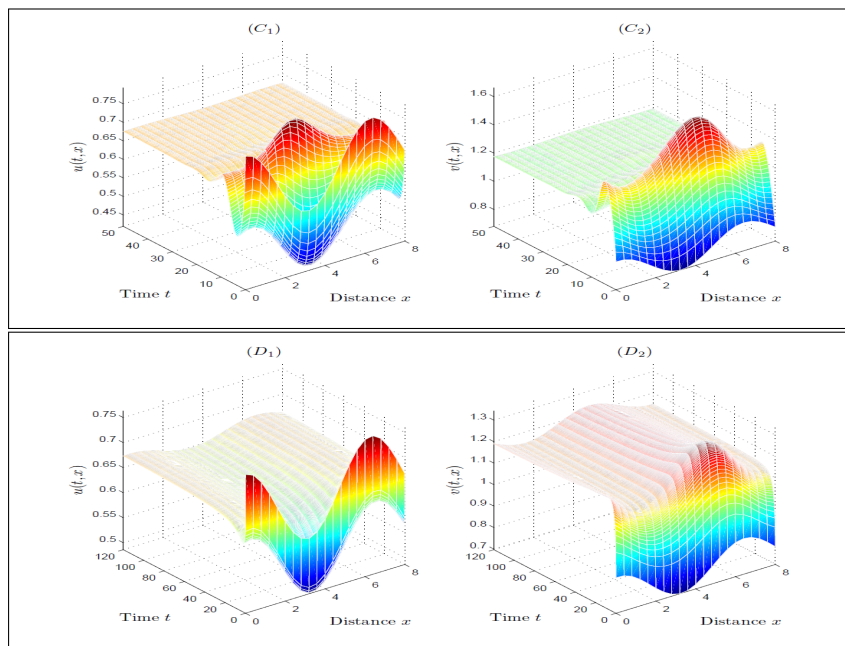


Figure 3.22: The numerical solution of time-fractional Schnackenberg model by MOL

CHAPTER

4

COUPLED REACTION-DIFFUSION SYSTEMS ON TIME-VARYING SPATIAL DOMAINS

“Tell me - a nut-cracker mathematician exclaims - just tell me in rigorous mathematical terms what the main problem in embryology is, and I will solve it.

OK, here is the problem: What is the mathematical formulation of the main problem(s) in embryology?”

Micha Gromov (see [16])

Since the spatial domains in several fields (e.g. biomathematics) are living organisms (cells). In this context, the evolution of the spatial domain in which interactions (changes) take place is a basic concept for understanding the dynamics of models. Thus, a good illustration of reaction-diffusion models must include the evolution of the spatial domain (cf. [15, 64]). This chapter is a partial contribution to answering the open question about the global existence of solutions for reaction-diffusion systems on a class of time-varying spatial domains, as well as the behavior of solutions. The results appearing in this context have been published through [32, 33].

4.1 Formulation of reaction-diffusion systems on isotropically evolving spatial domains

Let Ω_t is a subset of \mathbb{R}^N with ($N \in \mathbb{N}$), where it satisfies the following properties: bounded, simply connected, time-varying, and its moving boundary $\partial\Omega_t$ has some smoothness. Through to a suitable C^l -diffeomorphism ($l \geq 2$) $\rho_t : \Omega_0 \rightarrow \Omega_t$, the time-varying domain Ω_t can be reffered into a static domain Ω_0 (see Figure 1.1). Furthermore, we assume that the diffeomorphism ρ_t is to be a C^2 map with respect to the variable t . Flow velocity $\vartheta(x, t)$ resulting from the change in the volume (over time) of domain Ω_t generates two extra terms ($\vartheta \cdot \nabla u$, and $u(\nabla \cdot \vartheta)$ which are called an advection term and a dilution term, respectively) to the equations of classical reaction–diffusion model, for more details (see sub-sub-section 1.3.2). In the present chapter, we deal with some classes of semilinear parabolic equations on a class of evolving domains, which take all along this chapter, the following basic assumptions:

(EDA1) The flow velocity $\vartheta(x, t)$, given by

$$\vartheta = \frac{dx}{dt}. \quad (4.1)$$

(EDA2) Isotropic domain deformation, i.e., the diffeomorphism Ξ_t , satisfies (for $T > 0$)

$$\rho_t(y) = x = \chi(t)y, \quad y = (y_1, \dots, y_N) \in \Omega_0, \quad t \in [0, T], \quad (4.2)$$

with $\chi \in C^2(\mathbb{R}_+; \mathbb{R}_+^*)$, moreover $\chi(0) = 1$.

Remark 4.1.1. Thanks to the assumptions (EDA1)-(EDA2), the flow velocity ϑ has the following explicit form

$$\vartheta(x, t) = \frac{\dot{\chi}(t)}{\chi(t)}x, \quad x \in \Omega_t, \quad t \in [0, T], \quad (4.3)$$

where $\dot{\chi}(t) := \frac{d\chi(t)}{dt}$. Thus, the divergence of the flow velocity ϑ is given by

$$\nabla \cdot \vartheta = N \frac{\dot{\chi}(t)}{\chi(t)}. \quad (4.4)$$

By means the diffeomorphism ρ_t , each function u_i ($i = 1, \dots, m$) of the system (1.39) can be mapped as a new function \bar{u}_i with the following relation:

$$\bar{u}_i(y, t) := u_i(\rho_t(y), t) = u_i(x, t), \quad i = 1, \dots, m, \quad (4.5)$$

where $(\bar{u}_i)_{i=1}^m =: \bar{u}$. Then, for each $i = 1, \dots, m$

$$\frac{\partial u_i}{\partial t} = \frac{\partial \bar{u}_i}{\partial t} + \nabla \bar{u} \cdot \frac{\partial \rho_t^{-1}(x)}{\partial t} = \frac{\partial \bar{u}_i}{\partial t} - \vartheta \cdot \nabla u_i, \quad (4.6)$$

$$\nabla \cdot (\vartheta u_i) = \vartheta \cdot \nabla u_i + u_i (\nabla \cdot \vartheta) = \vartheta \cdot \nabla u_i + N \frac{\dot{\chi}(t)}{\chi(t)} \bar{u}_i, \quad (4.7)$$

$$\Delta u_i = \sum_{j=1}^N \mathcal{H}_y \bar{u}_i \frac{\partial \rho_t^{-1}(x)}{\partial x_j} \cdot \frac{\partial \rho_t^{-1}(x)}{\partial x_j} + \nabla \bar{u}_i \cdot \frac{\partial^2 \rho_t^{-1}(x)}{\partial x_j^2} = \frac{1}{\chi^2(t)} \Delta \bar{u}_i, \quad (4.8)$$

where ρ_t^{-1} denotes the inverse of ρ_t with respect to the spatial variable, and $\mathcal{H}_y \bar{u}_i$ denotes the Hessian matrix of \bar{u}_i (for $i = 1, \dots, m$). Therefore, the system (1.39) (suppose that $f(x, t, u) = f(u) := (f_i(u))_{i=1}^m$) is transformed in equivalent way into the auxiliary reaction-diffusion system in the static reference domain Ω_0 :

$$\begin{cases} \frac{\partial \bar{u}_i}{\partial t} - \frac{d_i}{\chi^2} \Delta \bar{u}_i = f_i(\bar{u}) - N \frac{\dot{\chi}}{\chi} \bar{u}_i & \text{in } \Omega_0 \times (0, T], i = 1, \dots, m, \\ \frac{\partial \bar{u}_i}{\partial \nu} = 0 & \text{on } \partial \Omega_0 \times \{t > 0\}, i = 1, \dots, m, \\ \bar{u}_i(y, 0) = \bar{u}_{0i}(y) & \text{on } \bar{\Omega}_0, i = 1, \dots, m. \end{cases} \quad (4.9)$$

By using the following change of variables (cf. [55]):

$$\varrho(t) := \int_0^t \frac{ds}{\chi^2(s)}, \quad (4.10)$$

and $\hat{u}_i(y, \varrho) := \bar{v}_i(y, t)$, within system (4.9). Then, the system (1.39) is equivalent to the following reaction-diffusion system in the static reference domain Ω_0 :

$$\begin{cases} \frac{\partial \hat{u}_i}{\partial t} - d_i \Delta \hat{u}_i = \chi^2 f_i(\hat{u}) - N \dot{\chi} \chi \hat{u}_i & \text{in } \Omega_0 \times (0, \bar{T}], i = 1, \dots, m, \\ \frac{\partial \hat{u}_i}{\partial \nu} = 0 & \text{on } \partial \Omega_0 \times \{t > 0\}, i = 1, \dots, m, \\ \hat{u}_i(y, 0) = \hat{u}_{0i}(y) & \text{on } \bar{\Omega}_0, i = 1, \dots, m, \end{cases} \quad (4.11)$$

where $(\hat{u}_i)_{i=1}^m =: \hat{u}$, $\bar{T} = \varrho(T)$, and we have used (without ambiguity) the fact $\varrho(t) = t$.

4.2 Global existence for activator-inhibitor reaction-diffusion systems on a class of evolving domains

The aim of this section is to give a positive answer to the open question about the global existence, uniqueness and uniform boundedness of solution for Gierer-Meinhardt system on spatially linear isotropically evolving domain.

4.2.1 Formulation of coupled activator-inhibitor reaction-diffusion systems on time-varying spatial domains

In this section we deal with the Gierer-Meinhardt type system on a time-varying domain which takes the following form:

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} + \nabla \cdot (\vartheta u) - d_1 \Delta u = \sigma_1 - \mu_1 u + \rho_1(u, v) \frac{u^p}{v^q} & \text{in } \Omega_t \times (0, T], \\ \frac{\partial v}{\partial t} + \nabla \cdot (\vartheta v) - d_2 \Delta v = \sigma_2 - \mu_2 v + \rho_2(u, v) \frac{u^r}{v^s} & \text{in } \Omega_t \times (0, T], \\ \frac{\partial u}{\partial \nu}(x, t) = \frac{\partial v}{\partial \nu}(x, t) = 0 & \text{on } \partial\Omega_t \times \{t > 0\}, \\ u(y, 0) = u_0(y), v(y, 0) = v_0(y) & \text{on } \bar{\Omega}_0, \end{array} \right. \quad (4.12)$$

where $T > 0$, $u := u(x, t)$, $v := v(x, t)$, $x := x(t) = (x_1(t), \dots, x_N(t))$, with ν being the unit outer normal to $\partial\Omega_t$, $p > 1$, $\sigma_2, s \geq 0$, $q, r, \sigma_1, \mu_i, d_i > 0$, $\rho_i \in C^1(\mathbb{R}_+^2; \mathbb{R}_+)$ ($i = 1, 2$). All along the sub-section, we will use the following assumptions:

(A1) The flow velocity $\vartheta(x, t)$ is identical to the domain velocity, i.e., $\vartheta = \frac{dx}{dt}$.

(A2) Isotropic domain deformation, i.e., the diffeomorphism Ξ_t satisfies

$$x = \Xi_t(y) = \chi(t)y, \quad y \in \Omega_0, \quad x \in \Omega_t, \quad t \in [0, T], \quad (4.13)$$

where $\chi \in C^2(\mathbb{R}_+; \mathbb{R}_+^*)$, and $\chi(0) = 1$.

(A3) There exist $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3 > 0$, such that

$$\mathcal{C}_1 \leq Y_i(t) := \mu_i \chi^2(t) + N \chi(t) \frac{d\chi(t)}{dt} \leq \mathcal{C}_2, \quad \forall t \in [0, \mathcal{T}), \mathcal{T} > 0 \quad (i = 1, 2), \quad (4.14)$$

and

$$\chi(t) \geq \mathcal{C}_3, \quad \forall t > 0. \quad (4.15)$$

$$(A4) \quad \frac{p-1}{r} < \min\left(\frac{q}{s+1}, 1\right).$$

(A5) There exist $\underline{\rho}_i, \bar{\rho}_i > 0$ ($i = 1, 2$), such that

$$\underline{\rho}_i \leq \rho_i(w_1, w_2) \leq \bar{\rho}_i, \quad w_i \geq 0 \quad (i = 1, 2). \quad (4.16)$$

Remark 4.2.1. If the domain growth function χ has positive derivative (e.g. logistic function which is feasible in biology) then for any $\mu_1, \mu_2 \in \mathbb{R}_+^*$ satisfy the assumption (A3).

By means the diffeomorphism ρ_t , u and v can be mapped as a new functions with the following definition:

$$\bar{u}(y, t) := u(\Xi_t(y), t) = u(x, t), \quad \bar{v}(y, t) := v(\Xi_t(y), t) = v(x, t). \quad (4.17)$$

Then, similar to (4.5)-(4.8) the system (4.12) can be transformed in equivalent way into the auxiliary reaction-diffusion system in the static reference domain Ω_0 :

$$\left\{ \begin{array}{l} \frac{\partial \bar{u}}{\partial t} - \frac{d_1}{\chi^2(t)} \Delta \bar{u} = \sigma_1 - \left(\mu_1 + N \frac{\dot{\chi}(t)}{\chi(t)} \right) \bar{u} + \rho_1(\bar{u}, \bar{v}) \frac{\bar{u}^p}{\bar{v}^q} \quad \text{in } \Omega_0 \times (0, T], \\ \frac{\partial \bar{v}}{\partial t} - \frac{d_2}{\chi^2(t)} \Delta \bar{v} = \sigma_2 - \left(\mu_2 + N \frac{\dot{\chi}(t)}{\chi(t)} \right) \bar{v} + \rho_2(\bar{u}, \bar{v}) \frac{\bar{u}^r}{\bar{v}^s} \quad \text{in } \Omega_0 \times (0, T], \\ \frac{\partial \bar{u}}{\partial \nu}(y, t) = \frac{\partial \bar{v}}{\partial \nu}(y, t) = 0 \quad \text{on } \partial\Omega_0 \times \{t > 0\}, \\ \bar{u}(y, 0) = u_0(y), \bar{v}(y, 0) = v_0(y) \quad \text{on } \bar{\Omega}_0. \end{array} \right. \quad (4.18)$$

By using the change of variables (4.10), and

$$\hat{u}(y, \varrho) := \bar{u}(y, t), \quad \hat{v}(y, \varrho) := \bar{v}(y, t), \quad (4.19)$$

within system (4.18). Then, the system (4.12) is equivalent to the following reaction-diffusion system in the fixed reference domain Ω_0 :

$$\left\{ \begin{array}{l} \frac{\partial \hat{u}}{\partial t} - d_1 \Delta \hat{u} = \sigma_1 \chi^2(t) + \chi^2(t) \rho_1(\hat{u}, \hat{v}) \frac{\hat{u}^p}{\hat{v}^q} - Y_1(t) \hat{u} =: F(\hat{u}, \hat{v}) \quad \text{in } \Omega_0 \times (0, \bar{T}], \\ \frac{\partial \hat{v}}{\partial t} - d_2 \Delta \hat{v} = \sigma_2 \chi^2(t) + \chi^2(t) \rho_2(\hat{u}, \hat{v}) \frac{\hat{u}^r}{\hat{v}^s} - Y_2(t) \hat{v} =: G(\hat{u}, \hat{v}) \quad \text{in } \Omega_0 \times (0, \bar{T}], \\ \frac{\partial \hat{u}}{\partial \nu}(y, t) = \frac{\partial \hat{v}}{\partial \nu}(y, t) = 0 \quad \text{on } \partial\Omega_0 \times \{t > 0\}, \\ \hat{u}(y, 0) = u_0(y), \hat{v}(y, 0) = v_0(y) \quad \text{on } \bar{\Omega}_0, \end{array} \right. \quad (4.20)$$

where $\bar{T} = \varrho(T)$, and without ambiguity we have used the fact $t := \varrho$.

4.2.2 Local existence and uniqueness of lower-bounded solution

Since the nonlinearity (F, G) is continuously differentiable on $\mathbb{R}_+ \times \mathbb{R}_+^*$ and by suppose that $u_0, v_0 \in L^\infty(\Omega_0)$. It is a classical task to show the existence of a unique local nonnegative classical solution of system (4.20) on $[0, \bar{T}_{max})$, where \bar{T}_{max} is the eventual blowing-up time in $L^\infty(\Omega_0)$ (see e.g. [46, 92]). By the equivalence of the systems (4.12) and (4.20), we get to the following result

Theorem 4.2.1. Suppose that $u_0, v_0 \in L^\infty(\Omega_0)$, and (A1)-(A2) are satisfied. Then the system (4.12) admits a unique classical solution (u, v) on $\Omega_t \times [0, T_{max})$, where $0 < T_{max} \leq \infty$. Moreover,

$$\text{if } T_{max} < \infty, \text{ then } \lim_{t \rightarrow T_{max}} (\|u(\cdot, t)\|_{L^\infty(\Omega_t)} + \|v(\cdot, t)\|_{L^\infty(\Omega_t)}) = +\infty. \quad (4.21)$$

The following result follows from the comparison principle.

Corollary 4.2.1. Under the same assumptions given in Theorem 4.2.1, in addition (A2) and $u_0, v_0 > 0$ hold. Then there exists $\mathcal{C} > 0$, such that

$$\hat{u}(y, t), \hat{v}(y, t) \geq \mathcal{C}, \quad \forall y \in \bar{\Omega}_0, \quad \forall t \in (0, \bar{T}_{max}). \quad (4.22)$$

Remark 4.2.2. Since the systems (4.12) and (4.20) are equivalent, then we have the same result of Corollary 4.2.1 for the solution of system (4.12).

4.2.3 Existence of global solution

To prove the global existence of solution for system (4.12), it suffices to prove the global existence of solution for system (4.20). Thus our task amounts to establish a uniform boundedness of $\|\tilde{u}(\cdot, t)\|_\infty$ and $\|\hat{v}(\cdot, t)\|_\infty$ on $[0, \bar{T}_{max})$. to do that is enough to derive a uniform estimate for $\left\| \frac{\tilde{u}^p}{\hat{v}^q} \right\|_{L^\tau(\Omega_0)}$ on $[0, \bar{T}_{max})$ for some $\tau > \frac{N}{2}$. For this purpose, we use the following candidate Lyapunov functional:

$$\mathcal{L}(t) = \int_{\Omega_0} \frac{\hat{u}^\alpha}{\hat{v}^\beta} dy, \quad (4.23)$$

where

(A6) α and β are positive constants, such that

$$\alpha \geq 2 \max\left(1, \frac{\mathcal{C}_2}{\mathcal{C}_1}\right), \quad \text{and} \quad \frac{2d_1d_2}{(d_1+d_2)^2} \geq \beta. \quad (4.24)$$

Now we are ready to state the main result and the proof will be mentioned later after some preparatory.

Theorem 4.2.2. We assume that the conditions (A1)-(A5) hold, in addition $u_0, v_0 \in L^\infty(\Omega_0)$, and $u_0, v_0 > 0$, then the solution of the system (4.12) is global and uniformly bounded.

The proof of Theorem 4.2.2 based on the following results.

Lemma 4.2.1. Let p, q, r, s the same parameters of system (4.12) satisfy (A4). For all $\alpha, \beta, \gamma, \varepsilon > 0$, there exist $\mathcal{K} := \mathcal{K}(\alpha, \beta, \gamma), \delta > 0$ and $\theta := \theta(\alpha) \in (0, 1)$, such that

$$\alpha \frac{w^{p+\alpha-1}}{z^{q+\beta}} \leq \varepsilon \beta \frac{w^{r+\alpha}}{z^{s+\beta+1}} + \varepsilon^{-\delta} \mathcal{K} \left(\frac{w^\alpha}{z^\beta} \right)^\theta, \quad w \geq 0, \quad z \geq \gamma. \quad (4.25)$$

Proof. Following the footsteps the proof of [88, Lemma 33.11], and we use ε -Young's inequality instead of Young's inequality. ■

Proposition 4.2.1. Let (\hat{u}, \hat{v}) the solution of (4.20) on $\Omega_0 \times [0, \bar{T}_{max}]$. We assume that the conditions (A1)-(A6) hold, then there exists a positive constant \hat{C} such that the functional \mathcal{L} satisfies

$$\mathcal{L}(t) \leq \hat{C}, \quad \forall t \in [0, \bar{T}_{max}]. \quad (4.26)$$

Proof. Let $\bar{T}^* \in (0, \bar{T}_{max})$. By using the homogeneous Neumann conditions on the boundary and the Green's formula, we get

$$\frac{d}{dt} \mathcal{L}(t) = \mathcal{I}_1 + \mathcal{I}_2 + \int_{\Omega_0} \mathcal{Q}(\hat{v} \nabla \hat{u}, \hat{u} \nabla \hat{v}) \frac{\hat{u}^{\alpha-2}}{\hat{v}^{\beta+2}} dy, \quad (4.27)$$

where the notations above represent

$$\begin{aligned}\mathcal{I}_1 &= -\alpha Y_1(t) \mathcal{L}(t) + \alpha \sigma_1 \chi^2(t) \int_{\Omega_0} \frac{\hat{u}^{\alpha-1}}{\hat{v}^\beta} dy + \alpha \chi^2(t) \int_{\Omega_0} \rho_1(\hat{u}, \hat{v}) \frac{\hat{u}^{p+\alpha-1}}{\hat{v}^{q+\beta}} dy, \\ \mathcal{I}_2 &= \beta Y_2(t) \mathcal{L}(t) - \beta \sigma_2 \chi^2(t) \int_{\Omega_0} \frac{\hat{u}^\alpha}{\hat{v}^{\beta+1}} dy - \beta \chi^2(t) \int_{\Omega_0} \rho_2(\hat{u}, \hat{v}) \frac{\hat{u}^{r+\alpha}}{\hat{v}^{s+\beta+1}} dy, \\ \mathcal{Q}(\hat{v} \nabla \hat{u}, \hat{u} \nabla \hat{v}) &= -\alpha(\alpha-1) d_1 \hat{v}^2 |\nabla \hat{u}|^2 + \alpha \beta (d_1 + d_2) \hat{v} \nabla \hat{u} \cdot \hat{u} \nabla \hat{v} - \beta(\beta+1) d_2 \hat{u}^2 |\nabla \hat{v}|^2,\end{aligned}$$

\mathcal{Q} is a quadratic form with respect to $\hat{v} \nabla \hat{u}$ and $\hat{u} \nabla \hat{v}$, in the light of assumption (A6) $\mathcal{Q}(\hat{v} \nabla \hat{u}, \hat{u} \nabla \hat{v})$ is nonpositive, thus we obtain

$$\frac{d}{dt} \mathcal{L}(t) \leq \mathcal{I}_1 + \mathcal{I}_2 =: \mathcal{I}. \quad (4.28)$$

On the other hand, thanks to the assumptions (A3) and (A5), we get

$$\mathcal{I} \leq (-\alpha \mathcal{C}_1 + \beta \mathcal{C}_2) \mathcal{L}(t) + \alpha \sigma_1 \bar{\chi} \int_{\Omega_0} \frac{\hat{u}^{\alpha-1}}{\hat{v}^\beta} dy + \int_{\Omega_0} \mathcal{R}(\hat{u}, \hat{v}) dy, \quad (4.29)$$

where $\bar{\chi} := \max_{t \in [0, \bar{T}^*]} \chi^2(t)$, and

$$\mathcal{R}(\hat{u}, \hat{v}) := \bar{\chi} \alpha \bar{\rho}_1 \frac{\hat{u}^{p+\alpha-1}}{\hat{v}^{q+\beta}} - \beta \mathcal{C}_3^2 \bar{\rho}_2 \frac{\hat{u}^{r+\alpha}}{\hat{v}^{s+\beta+1}}. \quad (4.30)$$

By virtue of Corollary 4.2.1 and Lemma 4.2.1 with $\varepsilon = \frac{\mathcal{C}_3^2 \bar{\rho}_2}{\bar{\rho}_1 \bar{\chi}}$ (taking into account the assumptions made), we get

$$\mathcal{R}(\hat{u}, \hat{v}) \leq \bar{\rho}_1 \bar{\chi} \varepsilon^{-\delta} \mathcal{K} \left(\frac{\hat{u}^\alpha}{\hat{v}^\beta} \right)^\theta, \quad (4.31)$$

where the constants $\delta, \mathcal{K} > 0$ and $\theta \in (0, 1)$ are mentioned in Lemma 4.2.1. Estimate (4.28) can be expressed by (4.29)-(4.31), as follows

$$\frac{d}{dt} \mathcal{L}(t) \leq (-\alpha \mathcal{C}_1 + \beta \mathcal{C}_2) \mathcal{L}(t) + \alpha \sigma_1 \bar{\chi} \int_{\Omega_0} \left(\frac{\hat{u}^\alpha}{\hat{v}^\beta} \right)^{\frac{\alpha-1}{\alpha}} \left(\frac{1}{\hat{v}^{\frac{\beta}{\alpha}}} \right) dy + \bar{\rho}_1 \bar{\chi} \varepsilon^{-\delta} \mathcal{K} \int_{\Omega_0} \left(\frac{\hat{u}^\alpha}{\hat{v}^\beta} \right)^\theta dy, \quad (4.32)$$

By virtue of Corollary 4.2.1 and using Holder's inequality, we obtain

$$\frac{d}{dt} \mathcal{L}(t) \leq (-\alpha \mathcal{C}_1 + \beta \mathcal{C}_2) \mathcal{L}(t) + \mathcal{C}_3 \mathcal{L}(t)^{\frac{\alpha-1}{\alpha}} + \mathcal{C}_4 \mathcal{L}^\theta(t), \quad (4.33)$$

where $\mathcal{C}_3 := \frac{\alpha\sigma_1\bar{\chi}|\Omega_0|^{\frac{1}{\alpha}}}{\mathcal{C}_\alpha^{\frac{\beta}{\alpha}}}$, and $\mathcal{C}_4 := \bar{\rho}_1\bar{\chi}\left(\frac{\bar{\rho}_1\bar{\chi}}{\mathcal{C}_3^2\rho_2}\right)^\delta \mathcal{K}|\Omega_0|^{1-\theta}$. Thanks to the assumption (A6), we have $(-\alpha\mathcal{C}_1 + \beta\mathcal{C}_2) < 0$, on the other hand, since $\mathcal{C}_3, \mathcal{C}_4 > 0$, and $\theta, \frac{\alpha-1}{\alpha} \in (0, 1)$, then according to [67, Lemma 2.2], there exists a positive constants \widehat{C} satisfies the desired inequality (4.26). \blacksquare

Lemma 4.2.2. Let $(\widehat{u}, \widehat{v})$ the solution of system (4.20) on $\Omega_0 \times [0, \bar{T}_{max})$, then for $\tau \in [1, +\infty)$, we have

$$\frac{\widehat{u}^p}{\widehat{v}^q} \in L^\infty\left(\left(0, \bar{T}_{max}\right); L^\tau(\Omega_0)\right), \quad (4.34)$$

Proof. For sufficiently large α and thanks to the Young's inequality, furthermore to the Corollary 4.2.1, we obtain

$$\begin{aligned} \int_{\Omega_0} \frac{\widehat{u}^{p\tau}}{\widehat{v}^{q\tau}} dy &= \int_{\Omega_0} \left(\frac{\widehat{u}^{p\tau}}{\widehat{v}^{\frac{\beta p\tau}{\alpha}}} \right) \widehat{v}^{\frac{\beta p\tau}{\alpha} - q\tau} dy \\ &\leq \mathcal{L}(t) + \int_{\Omega_0} \frac{1}{\widehat{v}^{(\alpha q - \beta p)\tau(\alpha - p\tau)^{-1}}} dy \\ &\leq \widehat{C} + \frac{|\Omega_0|}{\mathcal{C}^{(\alpha q - \beta p)\tau(\alpha - p\tau)^{-1}}}, \end{aligned} \quad (4.35)$$

on $(0, \bar{T}_{max})$. Thus, the desired result is achieved. \blacksquare

Proof. (Theorem 4.1.2) Thanks to the transformations (4.17) and (4.19), it suffices to prove that the solution $(\widehat{u}, \widehat{v})$ of system (4.20) satisfies the following estimate:

$$\forall t \in (0, \bar{T}_{max}), \quad \|\widehat{u}(\cdot, t)\|_{L^\infty(\Omega_0)} + \|\widehat{v}(\cdot, t)\|_{L^\infty(\Omega_0)} \leq \mathcal{G}(t), \quad (4.36)$$

where $\mathcal{G} \in C(\mathbb{R}_+; \mathbb{R}_+)$. Indeed, thanks to the Lemma 4.2.2 and L^p -regularity theory for the heat operator; We get

$$\mathcal{C}_5 := \sup_{t \in (0, \bar{T}_{max})} \|\widehat{u}(\cdot, t)\|_{L^\infty(\Omega_0)} < \infty. \quad (4.37)$$

Let $\bar{T}^* \in (0, \bar{T}_{max})$, through the comparison principle, \widehat{v} is bounded from above by the solution \widehat{V} of the following initial-boundary value problem:

$$\begin{cases} \frac{\partial \widehat{V}}{\partial t} - d_1 \Delta \widehat{V} = \sigma_2 \bar{\chi} + \bar{\rho}_2 \bar{\chi} \mathcal{C}_{\widehat{u}, \widehat{v}} - \mathcal{C}_1 \widehat{V} & \text{in } \Omega_0 \times (0, \bar{T}^*), \\ \frac{\partial \widehat{V}}{\partial \nu}(y, t) = 0 & \text{on } \partial\Omega_0 \times \{t > 0\}, \\ \widehat{V}(y, 0) = \widehat{v}_0(y) & \text{on } \bar{\Omega}_0, \end{cases} \quad (4.38)$$

where $\mathcal{C}_{\widehat{u}, \widehat{v}} := \mathcal{C}_{\widehat{u}, \widehat{v}}(\mathcal{C}, \mathcal{C}_5) > 0$. Using again the L^p -regularity theory for the heat operator, we get

$$\sup_{t \in (0, \bar{T}^*)} \|\widehat{v}(\cdot, t)\|_{L^\infty(\Omega_0)} \leq \sup_{t \in (0, \bar{T}^*)} \|\widehat{V}(\cdot, t)\|_{L^\infty(\Omega_0)} < \infty. \quad (4.39)$$

According to (4.37) and (4.39), the assertion (4.36) holds, hence the proof is complete. ■

4.2.4 Examples and numerical experiments

In this sub-section, we consider as examples a special cases of system (4.12). We have used numerical analysis and Matlab computer simulation to obtain Figures for the aim to examine the theoretical results mentioned above in this chapter.

Example 4.2.1. In system (4.12) the parameters are selected as:

$$\begin{cases} \sigma_1 = 3 & \mu_1 = 5 & p = 2 & q = 1 \\ \sigma_2 = 2 & \mu_2 = 3 & r = 2 & s = 0 \end{cases}, \quad (4.40)$$

and

$$\rho_1(u, v) = \frac{10}{1 + 10^{-4} \times u^2}, \quad \rho_1(u, v) = \frac{1}{2}, \quad \forall u, v \in \mathbb{R}_+^*. \quad (4.41)$$

The logistic growth of domain's evolution function is considered:

$$\chi(t) = \frac{5}{1 + e^{(\ln(4)-t)}}, \quad \forall t \in \mathbb{R}_+, \quad (4.42)$$

with the initial data (for $y \in \Omega_0 := (1, 3) \subset \mathbb{R}$):

$$\begin{cases} u_0(y) = 2.8 - 0.03 \cos(y), \\ v_0(y) = 2.53 - 0.03 \cos(y). \end{cases} \quad (4.43)$$

It is not difficult to verify that the parameters (4.40) and the functions (4.41)-(4.43) satisfy the conditions of Theorem 4.2.2.

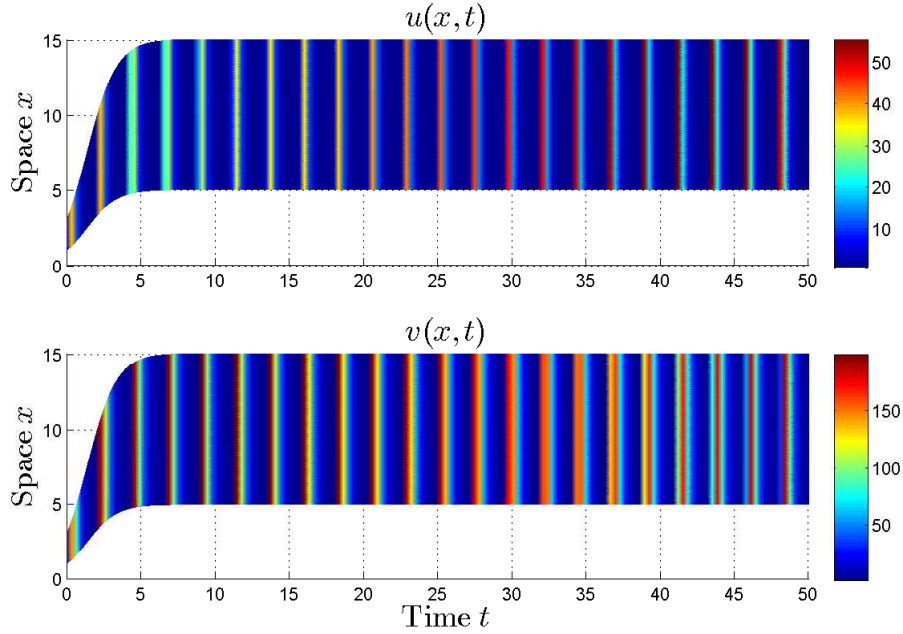


Figure 4.1: The approximate solution of system (4.12) on evolving domain $\Omega_t = (\chi(t), 3\chi(t))$, subject to the parameters in Example 1.

Figure 4.1 depicts the approximate solution of the system (4.12) in the case of evolving (logistic growth) domain according to the input (4.40)-(4.43), which confirms the theoretical existence and uniform boundedness results; Moreover, shows interesting vertical patterns.

Example 4.2.2. In system (4.12) the parameters are selected as:

$$\left\{ \begin{array}{cccc} \sigma_1 = 1 & \mu_1 = 9 & p = 2 & q = 2 \\ \sigma_2 = 0 & \mu_2 = 10 & r = 2 & s = 1 \end{array} \right\}, \quad (4.44)$$

and

$$\rho_1(u, v) = 3, \quad \rho_2(u, v) = 2, \quad \forall u, v \in \mathbb{R}_+^*. \quad (4.45)$$

The exponential growth of domain's evolution function is considered:

$$\chi(t) = e^{0.03t}, \quad \forall t \in \mathbb{R}_+, \quad (4.46)$$

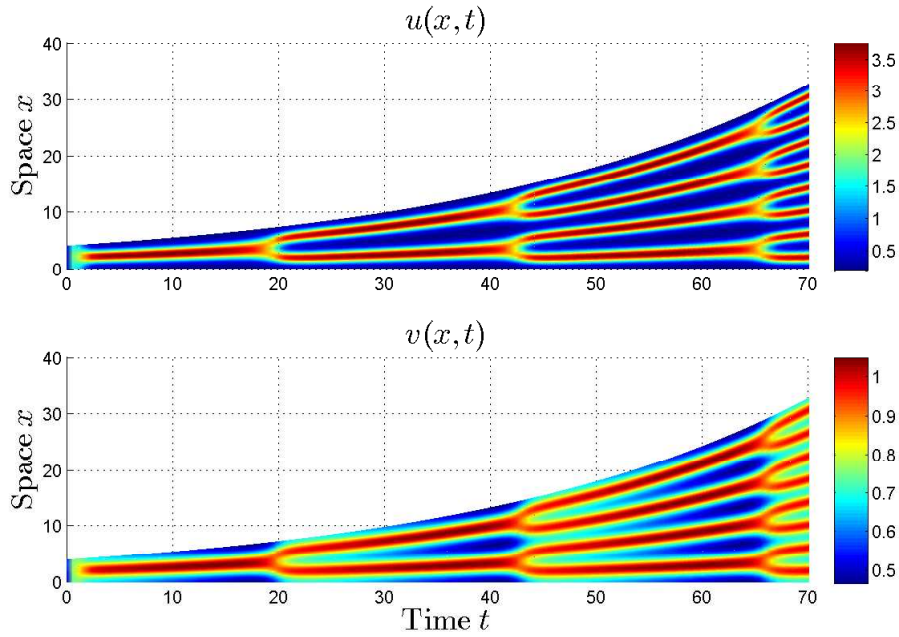


Figure 4.2: The approximate solution of system (4.12) on evolving domain $\Omega_t = (0, 4\chi(t))$, subject to the parameters in Example 2.

with the initial data (for $y \in \Omega_0 := (0, 4) \subset \mathbb{R}$):

$$\begin{cases} u_0(y) = 0.38 - 0.03 \cos(y), \\ v_0(y) = 0.53 - 0.03 \cos(y). \end{cases} \quad (4.47)$$

It is clear that the parameters (4.44) and the functions (4.45)-(4.47) satisfy the conditions of Theorem 4.2.2.

Figure 4.2 depicts the approximate solution of the system (4.12) in the case of evolving (exponential growth) domain according to the input (4.44)-(4.47), which confirms the theoretical existence and uniform boundedness results; Moreover, shows interesting horizontal patterns.

4.3 Global existence and asymptotic stability for a class of reaction-diffusion systems on growing domains

The main purpose of this section is to extend the result of A. Barabanova [10] on the global existence, uniqueness, uniform boundedness, and the asymptotic behavior of solutions for a weakly coupled class of reaction-diffusion systems on a growing domain with an isotropic growth, as well as numerical simulations are used to affirm and support the analytical findings.

4.3.1 Formulation of a class of coupled reaction-diffusion systems on growing domains

In this section, we study a class of reaction-diffusion systems on a growing domain, that take the form:

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} + \nabla \cdot (\partial u) - d_1 \Delta u + f(u, v) = 0 & \text{in } \Omega_t \times (0, T), \\ \frac{\partial v}{\partial t} + \nabla \cdot (\partial v) - d_2 \Delta v - f(u, v) = 0 & \text{in } \Omega_t \times (0, T), \\ \frac{\partial u}{\partial \nu}(x, t) = \frac{\partial v}{\partial \nu}(x, t) = 0 & \text{on } \partial \Omega_t \times (0, T), \\ u(y, 0) = u_0(y) \geq 0, v(y, 0) = v_0(y) \geq 0 & \text{in } \bar{\Omega}_0, \end{array} \right. \quad (4.48)$$

where $T > 0$, $x := x(t) = (x_1(t), \dots, x_N(t))$, ν is the unit outer normal to $\partial \Omega_t$, $d_1, d_2 > 0$, and the function $f \in C^1(\mathbb{R}_+^2; \mathbb{R}_+)$. According to [6, 45, 48], R. H. Martin posed the initial problem regarding the global existence of solutions on fixed domains when $f(u, v) = uv^r$. This gave rise to several interesting studies, with the a constraint on the initial data. Firstly, N. Alikakos [6] established the global existence and L^∞ -bounds of solutions for positive initial data and $1 \leq r \leq \frac{N+2}{N}$. This result was extended by K. Masuda [68] who showed that solutions to this system exist globally for all $r \geq 1$. A. Haraux and A. Youkana [45] generalized the method of K. Masuda to nonlinearities of the type $f(u, v) = u\psi(v)$ where

$$\lim_{\eta \rightarrow \infty} \frac{\log(1 + \psi(\eta))}{\eta} = 0.$$

Perhaps the greatest accomplishment in this respect was achieved by A. Barabanova [10] as she considered the condition $\psi(v) \leq e^{\alpha v}$. Her work included all the previous results regarding the global existence of solutions to system (4.48) on fixed domains for any dimension N . Other related results can be found in the literature taking into

consideration different forms of subgrowth nonlinearity with and without the addition of other diffusion terms including [81, 48, 52, 53, 89, 4, 90, 3, 29].

The studies discussed above deal only with fixed domains. The open question of the global existence of solutions for reaction-diffusion systems over time-varying domains (cf. [49]) has been partially answered by C. Venkataraman *et al.* [105]. Throughout this section, we impose the following assumptions:

(GDA1) The flow velocity $\vartheta(x, t)$ is identical to the domain velocity, i.e. $\vartheta = \frac{dx}{dt}$.

(GDA2) Isotropic domain deformation, i.e. the diffeomorphism ρ_t satisfies

$$x = \rho_t(y) = \chi(t)y, \quad y \in \Omega_0, \quad x \in \Omega_t, \quad t \geq 0. \quad (4.49)$$

(GDA3) $\chi \in C^2(\mathbb{R}_+; \mathbb{R}_+^*)$, $\chi(0) = 1$, and

$$\chi_d := \inf_{t \geq 0} \frac{d\chi(t)}{dt} > 0. \quad (4.50)$$

(GDA4) There exists a function $\varphi \in C^1(\mathbb{R}_+; \mathbb{R}_+)$, where $\varphi(0) = 0$, and a constant $\alpha > 0$ such that

$$f(\xi, \eta) \leq \varphi(\xi) e^{\alpha\eta}, \quad \forall (\xi, \eta) \in \mathbb{R}_+^2. \quad (4.51)$$

Remark 4.3.1. From assumptions (GDA1)-(GDA3), we note that the domain is ever growing over a period of time, which is the case in several natural phenomena such as the ones exhibiting linear or exponential growth.

By using the diffeomorphism ρ_t , functions u and v can be mapped as the new functions defined by:

$$\begin{aligned} \bar{u}(y, t) &:= u(\rho_t(y), t) = u(x, t), \\ \bar{v}(y, t) &:= v(\rho_t(y), t) = v(x, t). \end{aligned} \quad (4.52)$$

Then, similar to (4.5)-(4.8) the system (4.48) can be transformed in an equivalent way into the following auxiliary reaction-diffusion system on the static reference domain Ω_0 :

$$\left\{ \begin{array}{l} \frac{\partial \bar{u}}{\partial t} - \frac{d_1}{\chi^2(t)} \Delta \bar{u} + f(\bar{u}, \bar{v}) + N \frac{\dot{\chi}(t)}{\chi(t)} \bar{u} = 0 \quad \text{in } \Omega_0 \times (0, T), \\ \frac{\partial \bar{v}}{\partial t} - \frac{d_2}{\chi^2(t)} \Delta \bar{v} - f(\bar{u}, \bar{v}) + N \frac{\dot{\chi}(t)}{\chi(t)} \bar{v} = 0 \quad \text{in } \Omega_0 \times (0, T), \\ \frac{\partial \bar{u}}{\partial \nu}(y, t) = \frac{\partial \bar{v}}{\partial \nu}(y, t) = 0 \quad \text{on } \partial \Omega_0 \times (0, T), \\ \bar{u}(y, 0) = \bar{u}_0(y) \geq 0, \quad \bar{v}(y, 0) = \bar{v}_0(y) \geq 0 \quad \text{in } \bar{\Omega}_0. \end{array} \right. \quad (4.53)$$

By means the change of variables (4.10), and

$$\hat{u}(y, \varrho) := \bar{u}(y, t), \quad \hat{v}(y, \varrho) := \bar{v}(y, t), \quad (4.54)$$

within system (4.53). Thus, the system (4.48) is equivalent to the following reaction-diffusion system on static domain Ω_0 :

$$\left\{ \begin{array}{l} \frac{\partial \hat{u}}{\partial t} - d_1 \Delta \hat{u} = -\chi^2(t) f(\hat{u}, \hat{v}) - N \dot{\chi}(t) \chi(t) \hat{u} =: F(\hat{u}, \hat{v}) \quad \text{in } \Omega_0 \times (0, \bar{T}), \\ \frac{\partial \hat{v}}{\partial t} - d_2 \Delta \hat{v} = \chi^2(t) f(\hat{u}, \hat{v}) - N \dot{\chi}(t) \chi(t) \hat{v} =: G(\hat{u}, \hat{v}) \quad \text{in } \Omega_0 \times (0, \bar{T}), \\ \frac{\partial \hat{u}}{\partial \nu}(y, t) = \frac{\partial \hat{v}}{\partial \nu}(y, t) = 0 \quad \text{on } \partial \Omega_0 \times (0, \bar{T}), \\ \hat{u}(y, 0) = \hat{u}_0(y) \geq 0, \hat{v}(y, 0) = \hat{v}_0(y) \geq 0 \quad \text{in } \bar{\Omega}_0, \end{array} \right. \quad (4.55)$$

where $\bar{T} = \varrho(T)$. Note that without ambiguity we have used the fact that $t = \varrho(t)$.

4.3.2 Local existence and uniqueness of positive solution

According to the assumptions stated above, the nonlinearity (F, G) is quasi-positive, i.e. $F(0, \eta), G(\xi, 0) \geq 0$ for all $\xi, \eta \geq 0$. Hence, by supposing $\hat{u}_0, \hat{v}_0 \in L^\infty(\Omega_0)$, it is a classical task to show the existence of a unique local nonnegative classical solution of system (4.55) on $[0, \bar{T}_{max})$, where \bar{T}_{max} is the eventual blowing-up time in $L^\infty(\Omega_0)$ (see e.g. [46, 92]). The equivalence of systems (4.48) and (4.55) leads to the following result.

Theorem 4.3.1. Suppose that $u_0, v_0 \in L^\infty(\Omega_0; \mathbb{R}_+)$ and (GDA1)-(GDA4) are satisfied. System (4.48) admits a unique nonnegative classical solution (u, v) on $\Omega_t \times [0, T_{max})$, where $0 < T_{max} \leq \infty$. Moreover,

$$\text{if } T_{max} < \infty, \text{ then } \lim_{t \rightarrow T_{max}} (\|u(\cdot, t)\|_{L^\infty(\Omega_t)} + \|v(\cdot, t)\|_{L^\infty(\Omega_t)}) = +\infty. \quad (4.56)$$

By applying the comparison principle to the first equation of (4.55), the boundedness of $u(x, t)$ follows such that

$$0 \leq u(x, t) \leq \|u_0\|_\infty, \quad \forall (x, t) \in \Omega_t \times [0, T_{max}), \quad (4.57)$$

where $\|\cdot\|_\infty := \|\cdot\|_{L^\infty(\Omega_0; \mathbb{R}_+)}$. The following two Lemmas will become useful later on (cf. [3]).

Lemma 4.3.1. Let Φ and Ψ be two nonnegative continuous functions on \mathbb{R}_+ with

$$\lim_{\xi \rightarrow +\infty} \Phi(\xi) = +\infty.$$

Then, there exists a positive constant \mathcal{C} such that

$$\Psi(\xi)(1 - \Phi(\xi)) \leq \mathcal{C}, \quad \forall \xi \in \mathbb{R}_+. \quad (4.58)$$

Lemma 4.3.2. Denoting the solution of (4.55) by (\hat{u}, \hat{v}) , the following inequality holds:

$$\int_{\Omega_0} f(\hat{u}, \hat{v}) dy \leq -\frac{d}{dt} \int_{\Omega_0} \hat{u}(y, t) dy. \quad (4.59)$$

Proof. Integrating both sides of the first equation of (4.55) over Ω_0 and combining the result with the assumption (GDA3), yields the desired result. ■

4.3.3 Existence of global solution

To prove the global existence of solutions to the original system (4.48), it suffices to prove the global existence of solutions to the equivalent system (4.55). Hence, our task is to establish the uniform boundedness of $\|\hat{v}(\cdot, t)\|_\infty$ on $[0, \bar{T}_{max})$, to which end it is enough to derive a uniform estimate for $\|G(\hat{u}, \hat{v})\|_{L^p(\Omega_0)}$ on $[0, \bar{T}_{max})$ for some $p > \frac{N}{2}$. For this purpose, we suggest the candidate Lyapunov functional

$$\mathcal{L}(t) = \int_{\Omega_0} \left[\beta \hat{u} + e^{p\alpha \hat{v}} (\hat{v} + 1)^{p\sigma} (K - \hat{u})^{-\mu} \right] dx, \quad (4.60)$$

where $K, \alpha, \beta, \mu, \sigma$ and p are positive constants such that

$$\|u_0\|_\infty < K, \quad \mu < \mu^* := \frac{4d_1 d_2}{(d_1 - d_2)^2}, \quad \alpha < \frac{\mu}{Kp}, \quad \sigma \geq \frac{\mu^*(\mu + 1)}{p(\mu^* - \mu)}, \quad (4.61)$$

with $d_1 \neq d_2$ and β to be specified at a later stage.

Theorem 4.3.2. We assume that conditions (GDA1)-(GDA4) hold and that $u_0, v_0 \in L^\infty(\Omega_0; \mathbb{R}_+)$. Then, the solution of system (4.48) is global and uniformly bounded on $\Omega_t \times [0, \infty)$.

The proof of the theorem has been omitted as it is an immediate consequence of the following results.

Proposition 4.3.1. Let (\hat{u}, \hat{v}) be the solution of (4.55) on $[0, \bar{T}_{max}]$. Then, there exist two positive constants C_1 and C_2 such that the functional \mathcal{L} satisfies

$$\frac{d}{dt} \mathcal{L}(t) \leq -C_1 \mathcal{L}(t) + C_2, \quad \forall t \in [0, \bar{T}^*], \quad \bar{T}^* \in (0, \bar{T}_{max}). \quad (4.62)$$

Proof. Using Green's formula and homogeneous Neumann conditions, we get

$$\frac{d}{dt} \mathcal{L}(t) = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 - \int_{\Omega_0} \mathcal{Q}(\nabla \hat{u}, \nabla \hat{v}) e^{p\alpha \hat{v}} (\hat{v} + 1)^{p\sigma} (\mathbb{K} - \hat{u})^{-\mu-2} dx. \quad (4.63)$$

The notations used in this equality are defined as

$$\begin{aligned} \mathcal{I}_1 &= \beta \frac{d}{dt} \int_{\Omega_0} \hat{u}(y, t) dy, \\ \mathcal{I}_2 &= N \dot{\chi}(t) \chi(t) \int_{\Omega_0} \left[\frac{\mu \hat{u}}{\hat{u} - \mathbb{K}} - p \hat{v} (\sigma (\hat{v} + 1)^{-1} + \alpha) \right] e^{p\alpha \hat{v}} (\hat{v} + 1)^{p\sigma} (\mathbb{K} - \hat{u})^{-\mu} dx, \\ \mathcal{I}_3 &= \chi^2(t) \int_{\Omega_0} [p(\mathbb{K} - \hat{u})(\alpha + \sigma (\hat{v} + 1)^{-1}) - \mu] f(\hat{u}, \hat{v}) e^{p\alpha \hat{v}} (\hat{v} + 1)^{p\sigma} (\mathbb{K} - \hat{u})^{-\mu-1} dx, \end{aligned}$$

and

$$\begin{aligned} \mathcal{Q}(\nabla \hat{u}, \nabla \hat{v}) &= \mu(\mu + 1) d_1 |\nabla \hat{u}|^2 + \mu p (d_1 + d_2) (\alpha + \sigma (\hat{v} + 1)^{-1}) (\mathbb{K} - \hat{u}) \nabla \hat{u} \cdot \nabla \hat{v} \\ &\quad + p d_2 (p\alpha^2 + 2p\alpha\sigma (\hat{v} + 1)^{-1} + \sigma (p\sigma - 1) (\hat{v} + 1)^{-2}) (\mathbb{K} - \hat{u})^2 |\nabla \hat{v}|^2. \end{aligned}$$

Note that \mathcal{Q} is a binary quadratic form with respect to $\nabla \hat{u}$ and $\nabla \hat{v}$. In the light of (4.61), $\mathcal{Q}(\nabla \hat{u}, \nabla \hat{v})$ is nonnegative, which yields

$$\frac{d}{dt} \mathcal{L}(t) \leq \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3. \quad (4.64)$$

From (4.61) and Lemma 4.3.1, we get

$$\mathcal{I}_2 \leq -N \dot{\chi}(t) \chi(t) \mathcal{L}(t) + N \dot{\chi}(t) \chi(t) \int_{\Omega_0} [1 - p \hat{v} (\sigma (\hat{v} + 1)^{-1} + \alpha)] e^{p\alpha \hat{v}} (\hat{v} + 1)^{p\sigma} (\mathbb{K} - \hat{u})^{-\mu} dx, \quad (4.65)$$

$$\mathcal{I}_2 \leq -N \chi_d \mathcal{L}(t) + N \chi^* \tilde{\beta} |\Omega_0| (\mathbb{K} - \|u_0\|_\infty)^{-\mu}, \quad (4.66)$$

where $\tilde{\beta}$ is a positive constant and $\chi^* = \|\dot{\chi}\chi\|_{L^\infty([0, \bar{T}^*])}$. In addition,

$$\mathcal{I}_3 \leq \bar{\chi}^2 (K - \|u_0\|_\infty)^{-\mu-1} \int_{\Omega_0} [Kp\sigma - (\mu - Kp\alpha)(\hat{v} + 1)] e^{p\alpha\hat{v}} (\hat{v} + 1)^{p\sigma-1} f(\hat{u}, \hat{v}) dx, \quad (4.67)$$

$$\mathcal{I}_3 \leq \bar{\chi}^2 \hat{\beta} (K - \|u_0\|_\infty)^{-\mu-1} \int_{\Omega_0} f(\hat{u}, \hat{v}) dx, \quad (4.68)$$

where $\hat{\beta}$ is a positive constant and $\bar{\chi} = \|\chi\|_{L^\infty([0, \bar{T}^*])}$. By letting $\beta = \bar{\chi}^2 \hat{\beta} (K - \|u_0\|_\infty)^{-\mu-1}$ and applying Lemma 4.3.2 to (4.68), we obtain the inequality (4.62) where

$$C_1 = N\chi_d, \quad C_2 = N\chi^* \tilde{\beta} |\Omega_0| (K - \|u_0\|_\infty)^{-\mu}. \quad (4.69)$$

■

Corollary 4.3.1. Under the assumptions (GDA1)-(GDA4) and $\hat{u}_0, \hat{v}_0 \in L^\infty(\Omega_0; \mathbb{R}_+)$, the solution of system (4.55) is global and uniformly bounded on $[0, \bar{\varrho}]$, where

$$\bar{\varrho} := \lim_{t \rightarrow +\infty} \varrho(t). \quad (4.70)$$

Proof. When $d_1 = d_2$, simple use of the maximal principle yields the announced result. The case $d_1 \neq d_2$ is not as straight forward. According to (GDA4) and (4.57), there exists a positive constant $\tilde{\mathcal{C}}$ such that

$$\max\{\hat{v}, f(\hat{u}, \hat{v})\} \leq \tilde{\mathcal{C}} e^{\alpha\hat{v}}. \quad (4.71)$$

The differential inequality (4.62) gives us $\mathcal{L}(t) \leq \frac{C_2}{C_1} + \mathcal{L}(0)e^{-C_1 t}$ on $(0, \bar{T}_{max})$. Therefore, $G(\hat{u}, \hat{v}) \in L^\infty\left(\left(0, \bar{T}_{max}\right); L^p(\Omega_0)\right)$. By using the regularizing effect of the parabolic equation (cf. [46, 44]), we obtain $\hat{v} \in L^\infty\left(\left(0, \bar{T}_{max}\right); L^\infty(\Omega_0)\right)$. Then, together with (4.57), we conclude that the solution of (4.55) is global and uniformly bounded on $[0, \bar{\varrho}]$. ■

4.3.4 Asymptotic behavior of solutions

In this subsection, we have inspired by the literature [109]. We establish the global stability of solutions for system (4.53) based on the following Lyapunov function:

$$\mathcal{V}(t) = \frac{1}{2} \int_{\Omega_0} [\zeta \bar{u}^2 + 2\bar{u}\bar{v} + \bar{v}^2] dy, \quad (4.72)$$

where

$$\varsigma > \frac{(d_1 + d_2)^2}{4d_1d_2}. \quad (4.73)$$

We need to have the following two Lemmas.

Lemma 4.3.3. ([65]) For a uniformly isotropic growing domain, the divergence of the flow velocity is constant if and only if the growth function is exponential.

Lemma 4.3.4. Let (\bar{u}, \bar{v}) be a solution of system (4.53) satisfying $(\bar{u}_0, \bar{v}_0) \in (C^2(\bar{\Omega}_0))^2$. Then, there exist $\nu \in (0, 1)$ and $C^* > 0$, such that

$$\|\bar{u}(y, \cdot)\|_{C^{\nu+1}([1, \infty))} + \|\bar{v}(y, \cdot)\|_{C^{\nu+1}([1, \infty))} \leq C^*, \quad \forall y \in \bar{\Omega}_0, \quad (4.74)$$

and

$$\|\bar{u}(\cdot, t)\|_{C^{\nu+2}(\bar{\Omega}_0)} + \|\bar{v}(\cdot, t)\|_{C^{\nu+2}(\bar{\Omega}_0)} \leq C^*, \quad \forall t \geq 1. \quad (4.75)$$

Proof. By the well-known parabolic-type L^p and Schauder estimates and embedding theorems (see e.g. [56, 62, 110, 111]) we can get the desired results. \blacksquare

Now, we are ready to state the main result of this part.

Theorem 4.3.3. Assume that (GDA1)-(GDA4) hold, and let $(\bar{u}_0, \bar{v}_0) \in (C^2(\bar{\Omega}_0))^2$, we assume also the growth function is exponential. Then the constant steady state $(0, 0)$ of system (4.53) is globally asymptotically stable in the sense that

$$\lim_{t \rightarrow \infty} \|\bar{u}(\cdot, t)\|_{\infty} = \lim_{t \rightarrow \infty} \|\bar{v}(\cdot, t)\|_{\infty} = 0. \quad (4.76)$$

Proof. To prove that the equilibrium $(0, 0)$ of system (4.53) is globally asymptotically stable, we need to establish that $\mathcal{V}(t)$ is a Lyapunov function. First, clearly $\mathcal{V}(t)$ is positive definite function. By simple use of Green's formula and taking into account the Neumann conditions, we get

$$\begin{aligned} \frac{d}{dt} \mathcal{V}(t) &= \varsigma \int_{\Omega_0} \bar{u} \frac{\partial \bar{u}}{\partial t} dy + \int_{\Omega_0} \left(\frac{\partial \bar{u}}{\partial t} \bar{v} + \frac{\partial \bar{v}}{\partial t} \bar{u} \right) dy + \int_{\Omega_0} \bar{v} \frac{\partial \bar{v}}{\partial t} dy \\ &= \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 + \mathcal{I}_4, \end{aligned}$$

where

$$\begin{aligned}\mathcal{I}_1 &= -\varsigma \frac{d_1}{\chi^2(t)} \int_{\Omega_0} |\nabla \bar{u}|^2 dy - \varsigma \int_{\Omega_0} \bar{u} f(\bar{u}, \bar{v}) dy - \varsigma N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{u}^2 dy, \\ \mathcal{I}_2 &= -\frac{d_1}{\chi^2(t)} \int_{\Omega_0} \nabla \bar{u} \cdot \nabla \bar{v} dy - \int_{\Omega_0} \bar{v} f(\bar{u}, \bar{v}) dy - N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{u} \bar{v} dy, \\ \mathcal{I}_3 &= -\frac{d_2}{\chi^2(t)} \int_{\Omega_0} \nabla \bar{u} \cdot \nabla \bar{v} dy + \int_{\Omega_0} \bar{u} f(\bar{u}, \bar{v}) dy - N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{u} \bar{v} dy, \\ \mathcal{I}_4 &= -\frac{d_2}{\chi^2(t)} \int_{\Omega_0} |\nabla \bar{v}|^2 dy + \int_{\Omega_0} \bar{v} f(\bar{u}, \bar{v}) dy - N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{v}^2 dy.\end{aligned}$$

Then

$$\frac{d}{dt} \mathcal{V}(t) = \mathcal{I}_1 + \mathcal{I}_2,$$

where

$$\mathcal{I}_1 = -\frac{1}{\chi^2(t)} \int_{\Omega_0} \tilde{\mathcal{Q}}(\nabla \bar{u}, \nabla \bar{v}) dy, \quad (4.77)$$

$$\mathcal{I}_2 = (1 - \varsigma) \int_{\Omega_0} \bar{u} f(\bar{u}, \bar{v}) dy - 2N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{u} \bar{v} dy - \varsigma N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{u}^2 dy - N \frac{\dot{\chi}(t)}{\chi(t)} \int_{\Omega_0} \bar{v}^2 dy, \quad (4.78)$$

with

$$\tilde{\mathcal{Q}}(\nabla \bar{u}, \nabla \bar{v}) = \varsigma d_1 |\nabla \bar{u}|^2 + (d_1 + d_2) \nabla \bar{u} \cdot \nabla \bar{v} + d_2 |\nabla \bar{v}|^2.$$

According to (4.73), $\tilde{\mathcal{Q}}(\nabla \bar{u}, \nabla \bar{v})$ is nonnegative quadratic form. Hence

$$\mathcal{I}_1 \leq 0. \quad (4.79)$$

From (4.73) and by using Young's inequality, we get

$$\varsigma > \frac{(d_1 + d_2)^2}{4d_1 d_2} \geq 1, \quad (4.80)$$

taking into account that (GDA3), (4.80) and $\bar{u}, \bar{v}, f(\bar{u}, \bar{v}) \geq 0$ hold. Then

$$\mathcal{I}_2 \leq 0. \quad (4.81)$$

Thus, it follows from (4.79) and (4.81) that

$$\frac{d}{dt} \mathcal{V}(t) = \mathcal{I}_1 + \mathcal{I}_2 \leq 0. \quad (4.82)$$

From (4.77) and (4.82), we get

$$\frac{d}{dt} \mathcal{V}(t) \leq -\varsigma \int_{\Omega_0} \bar{u}^2 \nabla \cdot \partial dy - \int_{\Omega_0} \bar{v}^2 \nabla \cdot \partial dy. \quad (4.83)$$

By Lemma 4.3.3, there exists $c > 0$, such that

$$\frac{d}{dt} \mathcal{V}(t) \leq -\zeta c \int_{\Omega_0} \bar{u}^2 dy, \quad (4.84)$$

$$\frac{d}{dt} \mathcal{V}(t) \leq -c \int_{\Omega_0} \bar{v}^2 dy. \quad (4.85)$$

Integrating (4.84) and (4.85) from 1 to t , we get

$$\int_1^t \int_{\Omega_0} \bar{u}^2 dy ds \leq \frac{\mathcal{V}(1)}{\zeta c} < +\infty, \quad (4.86)$$

$$\int_1^t \int_{\Omega_0} \bar{v}^2 dy ds \leq \frac{\mathcal{V}(1)}{c} < +\infty. \quad (4.87)$$

Hence

$$\int_1^{+\infty} \int_{\Omega_0} \bar{u}^2 dy ds < +\infty, \quad (4.88)$$

$$\int_1^{+\infty} \int_{\Omega_0} \bar{v}^2 dy ds < +\infty. \quad (4.89)$$

From Lemma 4.3.4, we deduce

$$\lim_{t \rightarrow \infty} \int_{\Omega_0} \bar{u}^2 dy = \lim_{t \rightarrow \infty} \int_{\Omega_0} \bar{v}^2 dy = 0. \quad (4.90)$$

By the well-known Gagliardo-Nirenberg inequality there exists $\bar{\mathcal{C}} > 0$, such that

$$\|\bar{u}(\cdot, t)\|_{\infty} \leq \bar{\mathcal{C}} \left(\|\bar{u}(\cdot, t)\|_{W^{1,\infty}(\Omega_0)}^{\frac{N}{N+2}} \|\bar{u}(\cdot, t)\|_{L^2(\Omega_0)}^{\frac{2}{N+2}} + \|\bar{u}(\cdot, t)\|_{L^2(\Omega_0)} \right), \quad t > 0, \quad (4.91)$$

$$\|\bar{v}(\cdot, t)\|_{\infty} \leq \bar{\mathcal{C}} \left(\|\bar{v}(\cdot, t)\|_{W^{1,\infty}(\Omega_0)}^{\frac{N}{N+2}} \|\bar{v}(\cdot, t)\|_{L^2(\Omega_0)}^{\frac{2}{N+2}} + \|\bar{v}(\cdot, t)\|_{L^2(\Omega_0)} \right), \quad t > 0. \quad (4.92)$$

It then follows from (4.90)-(4.92) and Lemma 4.3.4, that (4.76) holds.

4.3.5 Examples and numerical experiments

In this sub-section, we consider as examples a special cases of system (4.48). We have used numerical analysis and a Matlab computer simulation to obtain Figures for the aim to examine the behavior of the system's solutions over time.

Example 4.3.1. The system parameters are selected as $T = 30000$, $(d_1, d_2) = (1, 2)$, $f(u, v) = 10u^6v^7$ (see [85]), and $\chi(t) = e^{10^{-4}t}$. The initial conditions are assumed to be

$$\begin{cases} u_0(y) = 1.905 + 0.09 \cos(4\pi y), \\ v_0(y) = 2.71 - 0.09 \sin(4\pi y). \end{cases}$$

Figures 4.3 and 4.4 depict the approximate solution of the system in the cases of fixed and time-varying domains, respectively. Figure 4.4 confirms the theoretical existence and uniform boundedness results presented in Theorem 4.3.2 with parameters

$$(\mathbb{K}, \mu, \mu^*, \alpha, p, \sigma) = (2, 7, 8, 3, 1.1, 60). \quad (4.93)$$

Also in Figure 4.4, we can observe that the solution (u, v) do converge towards to $(0, 0)$.

Example 4.3.2. The system parameters are selected as $T = 5000$, $(d_1, d_2) = (1, 3)$, $f(u, v) = 7ue^{\sqrt{3}v}$ (see [10]), and $\chi(t) = e^{3 \times 10^{-4}t}$. The initial conditions are assumed to be

$$\begin{cases} u_0(y) = 0.73 + 0.09 \cos(4\pi y), \\ v_0(y) = 0.93 - 0.09 \sin(4\pi y). \end{cases}$$

Figures 4.5 and 4.6 depict the approximate solutions of the system in the cases of fixed and variable domains, respectively. Figure 4.6 confirms the theoretical existence and uniform boundedness results presented in Theorem 4.3.2 with parameters

$$(\mathbb{K}, \mu, \mu^*, \alpha, p, \sigma) = (1, 2, 3, \sqrt{3}, 1.1, 10). \quad (4.94)$$

Also in Figure 4.6, we can observe that the solution (u, v) do converge towards to $(0, 0)$.

Example 4.3.3. The system parameters are selected as $T = 800$, $(d_1, d_2) = (1, 5)$, $\chi(t) = e^{5 \times 10^{-3}t}$, and $f(u, v) = u(u + v + 1)^{\sqrt{7}} e^{u^2 + 3v}$. The initial conditions are assumed to be

$$\begin{cases} u_0(y) = 0.07 + 0.02 \cos(2\pi y), \\ v_0(y) = 1.9 - 0.4 \sin(2\pi y). \end{cases}$$

Figures 4.7 and 4.8 depict the approximate solutions of the system in the cases of fixed and variable domains, respectively. Figure 4.8 confirms the theoretical existence and uniform boundedness results presented in Theorem 4.3.2 with parameters

$$(\mathbb{K}, \mu, \mu^*, \alpha, p, \sigma) = \left(0.1, 1, \frac{5}{4}, 5, \sqrt{3}, 6\right). \quad (4.95)$$

Also in Figure 4.8, we can observe that the solution (u, v) do converge towards to $(0, 0)$.

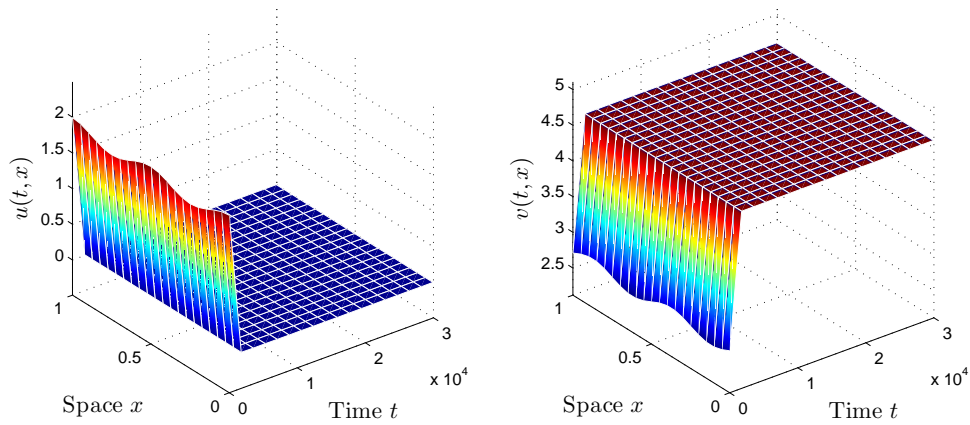


Figure 4.3: The approximate solution of system (4.48) on fixed domain $\Omega_0 = (0, 1)$, subject to the parameters in Example 1.

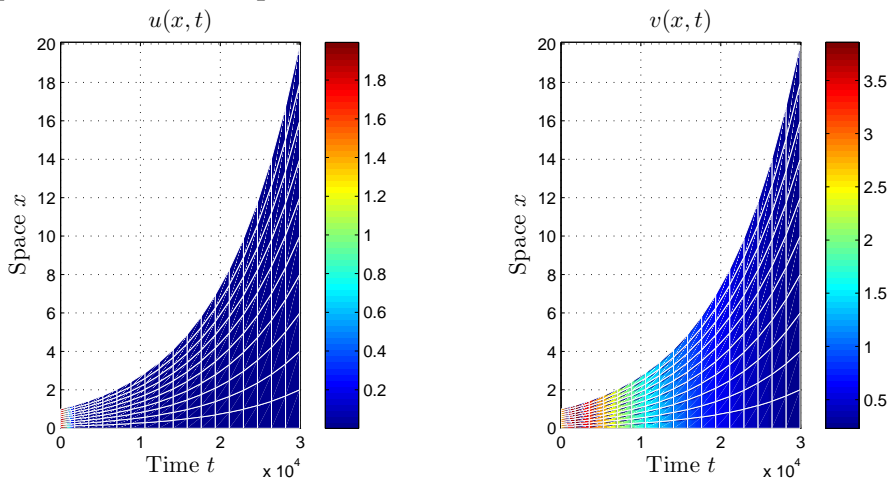


Figure 4.4: The approximate solution of system (4.48) on growing domain $\Omega_t = (0, \chi(t))$ where $t \in [0, T]$, subject to the parameters in Example 1.

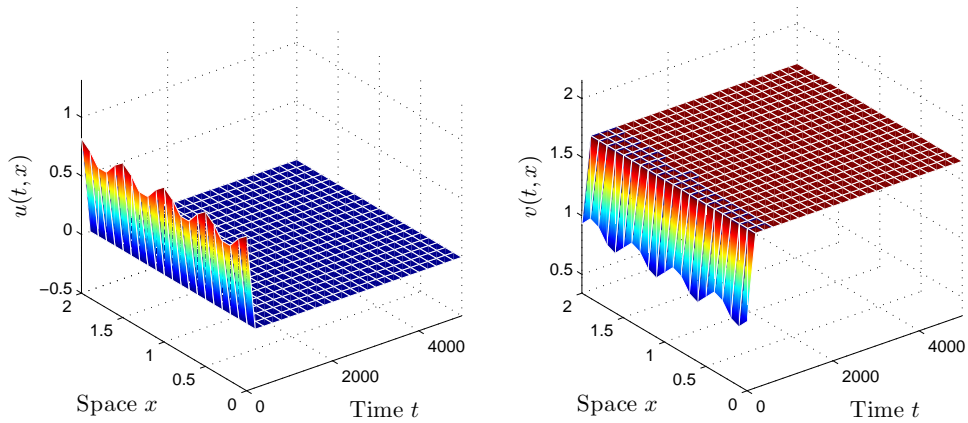


Figure 4.5: The approximate solution of system (4.48) on fixed domain $\Omega_0 = (0, 2)$, subject to the parameters in Example 2.

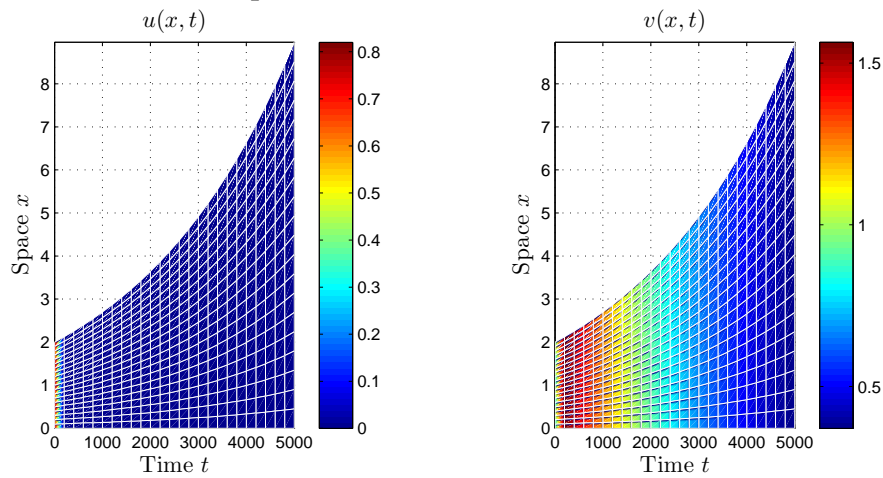


Figure 4.6: The approximate solution of system (4.48) on growing domain $\Omega_t = (0, 2\chi(t))$ where $t \in [0, T]$, subject to the parameters in Example 2.

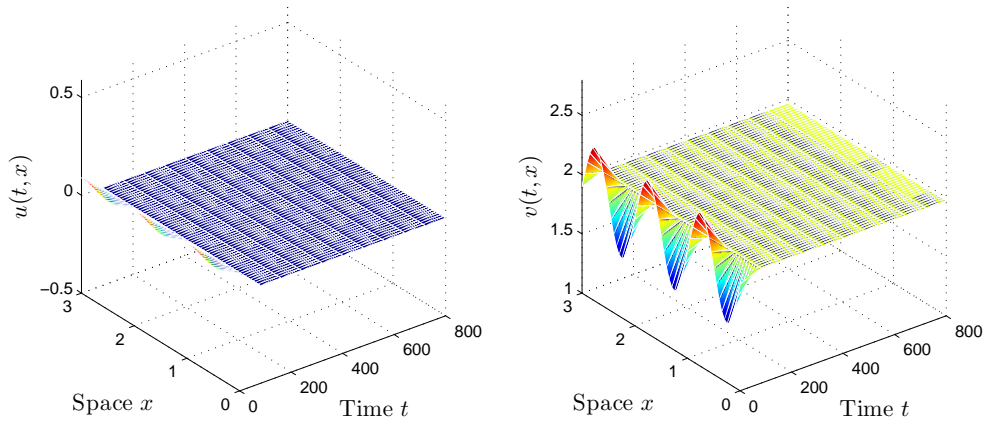


Figure 4.7: The approximate solution of system (4.48) on fixed domain $\Omega_0 = (0, 3)$, subject to the parameters in Example 3.

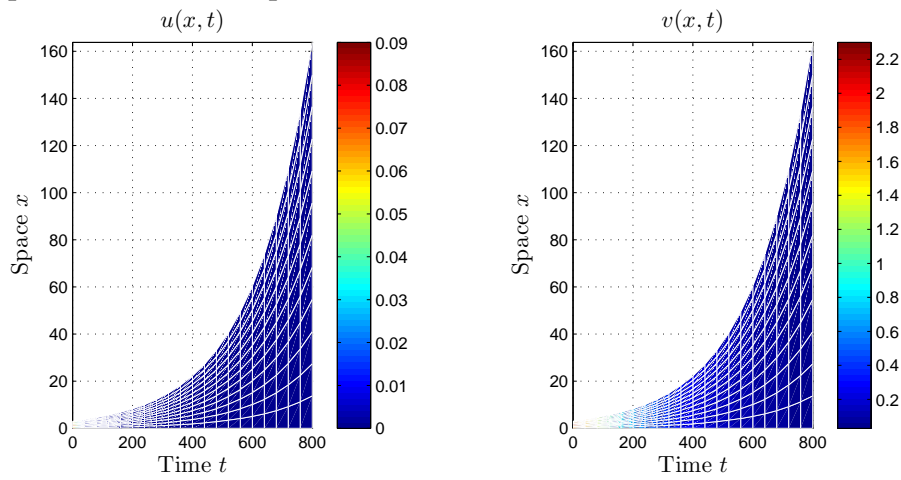


Figure 4.8: The approximate solution of system (4.48) on growing domain $\Omega_t = (0, 3\chi(t))$ where $t \in [0, T]$, subject to the parameters in Example 3.

4.4 Global existence and behavior of solutions for reaction-diffusion systems with more than exponential nonlinearity on growing domains

This section primarily seeks to extend the results of B. Rebiai and S. Benachour [89] on the global existence, uniqueness, uniform boundedness, and the asymptotic behavior of solutions for a weakly coupled reaction-diffusion systems with exponential nonlinearity on a growing domain with an isotropic growth, the desired results are obtained by using Lyapunov functions' method. The theoretical findings are supported and affirmed by numerical simulation.

4.4.1 Formulation of coupled reaction-diffusion systems with exponential nonlinearity on growing domains

In the present sub-section, we deal with a class of semilinear parabolic equations with exponential nonlinearity on a class of growing domains, which takes the form:

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} + \nabla \cdot (\vartheta u) - d_1 \Delta u + f_1(u, v) = 0 & \text{in } \mathcal{Q}_T(t), \\ \frac{\partial v}{\partial t} + \nabla \cdot (\vartheta v) - d_2 \Delta v - f_2(u, v) = 0 & \text{in } \mathcal{Q}_T(t), \\ \frac{\partial u}{\partial \nu}(x, t) = \frac{\partial v}{\partial \nu}(x, t) = 0 & \text{on } \Gamma_T(t), \\ u(y, 0) = u_0(y) \geq 0, v(y, 0) = v_0(y) \geq 0 & \text{in } \bar{\Omega}_0, \end{array} \right. \quad (4.96)$$

where $\mathcal{Q}_T(t) := \Omega_t \times (0, T)$, $\Gamma_T(t) := \partial\Omega_t \times (0, T)$, $T > 0$, $x := (x_1(t), \dots, x_N(t))$, ν is the unit outer normal to $\partial\Omega_t$, $d_1, d_2 > 0$, and $f_i \in C^1(\mathbb{R}_+^2; \mathbb{R}_+)$ ($i = 1, 2$) where $\mathbb{R}_+ := [0, +\infty)$.

The problem concerning the existence of global solutions of system (4.96) on static domain $\Omega := \Omega_0$ (when $f_1(u, v) = f_2(u, v) = uv^r$, $r > 0$) was proposed by R. H. Martin (cf. [6, 45, 48]). This has given rise to several of interesting investigations, among them: [6, 68, 44, 45, 72, 10, 53, 89, 3]. In [105] C. Venkataraman *et al.* have answered partially to the open problem regarding the existence of global solutions of reaction-diffusion equations on evolving domains. In their research, they proved the existence of unique global solution for n -components ($n \geq 2$) reaction-diffusion systems such that the reaction functions satisfying polynomial growth condition and other conditions attached to the Lyapunov-type function on bounded, isotropic, time-dependent domain for any spatial dimension N . On the other hand, when the reaction functions of system (4.96) have exponential growth, i.e.

$$f_1(\xi, \eta) = f_2(\xi, \eta) \leq \varphi(\xi) e^{\alpha\eta}, \quad \forall (\xi, \eta) \in \mathbb{R}_+^2,$$

(where $\varphi \in C^1(\mathbb{R}_+; \mathbb{R}_+)$, $\varphi(0) = 0$, and $\alpha > 0$) the existence of global solutions, uniform boundedness, as well as the asymptotic behavior of solutions for system (4.96) on a growing domain with an isotropic growth, they have been proved by R. Douaifia *et al.* (cf. [32]). Throughout the present section, we use the following notations: $\mathbb{R}_+ := [0, +\infty)$ and $\mathbb{R}_+^* := (0, +\infty)$, some conditions are imposed:

(A1) We assume that $\vartheta = \frac{dx}{dt}$ (i.e. the domain velocity equals the flow velocity).

(A2) The diffeomorphism ρ_t satisfies

$$x = \rho_t(y) = \chi(t)y, \quad y \in \Omega_0, \quad x \in \Omega_t, \quad t \geq 0. \quad (4.97)$$

i.e. the isotropic deformation of domain Ω_t over time.

(A3) $\chi \in C^2(\mathbb{R}_+)$, $\chi(t) > 0$ for all $t \geq 0$, $\chi(0) = 1$, and

$$\chi_d := \inf_{t \geq 0} \frac{d\chi(t)}{dt} > 0. \quad (4.98)$$

(A4) $f_1(0, \eta) = 0$, $\forall \eta \geq 0$.

(A5) There exists $\Psi \in C^1(\mathbb{R}_+; \mathbb{R}_+)$, and $\beta \geq 1$ where $\lim_{\eta \rightarrow +\infty} \eta^{\beta-1} \psi(\eta) = \ell \geq 0$, such that

$$f_2(\xi, \eta) \leq \Psi(\eta) f_1(\xi, \eta), \quad \forall (\xi, \eta) \in \mathbb{R}_+^2. \quad (4.99)$$

(A6) There exists $\varphi \in C^1(\mathbb{R}_+; \mathbb{R}_+)$, where $\varphi(0) = 0$, and a constant $\alpha > 0$, such that

$$f_2(\xi, \eta) \leq \varphi(\xi) e^{\alpha \eta^\beta}, \quad \forall (\xi, \eta) \in \mathbb{R}_+^2, \quad (4.100)$$

where β is the same as in (A5).

Remark 4.4.1. From the conditions (A1)-(A3) we note that the domain's evolution function χ is increasing function (e.g. exponential, linear growth, and others) which is appearing in several natural phenomena (e.g. the spread of epidemics, the expansion of the breeding area of bacteria, ect). Thanks to the diffeomorphism ρ_t , we can define new functions \bar{u} and \bar{v} related to u and v , as follows

$$\bar{u}(y, t) := u(\rho_t(y), t) = u(x, t), \quad (4.101)$$

$$\bar{v}(y, t) := v(\rho_t(y), t) = v(x, t).$$

Thus, the system (4.96) turns to the following system on static domain Ω_0 :

$$\left\{ \begin{array}{l} \frac{\partial \bar{u}}{\partial t} - \frac{d_1}{\chi^2(t)} \Delta \bar{u} + f_1(\bar{u}, \bar{v}) + N \frac{\dot{\chi}(t)}{\chi(t)} \bar{u} = 0 \quad \text{in } \mathcal{Q}_T(0), \\ \frac{\partial \bar{v}}{\partial t} - \frac{d_2}{\chi^2(t)} \Delta \bar{v} - f_2(\bar{u}, \bar{v}) + N \frac{\dot{\chi}(t)}{\chi(t)} \bar{v} = 0 \quad \text{in } \mathcal{Q}_T(0), \\ \frac{\partial \bar{u}}{\partial \nu}(x, t) = \frac{\partial \bar{v}}{\partial \nu}(x, t) = 0 \quad \text{on } \Gamma_T(0), \\ \bar{u}(y, 0) = \bar{u}_0(y), \bar{v}(y, 0) = \bar{v}_0(y) \quad \text{in } \bar{\Omega}_0. \end{array} \right. \quad (4.102)$$

Again, we need to do another transformation through the change of variables (4.10), and

$$\hat{u}(y, \varrho) := \bar{u}(y, t), \quad \hat{v}(y, \varrho) := \bar{v}(y, t), \quad (4.103)$$

within system (4.102), yields the following equivalent system on Ω_0 :

$$\left\{ \begin{array}{l} \frac{\partial \hat{u}}{\partial t} - d_1 \Delta \hat{u} = F_1(\hat{u}, \hat{v}) \quad \text{in } \mathcal{Q}_{\bar{T}}(0), \\ \frac{\partial \hat{v}}{\partial t} - d_2 \Delta \hat{v} = F_2(\hat{u}, \hat{v}) \quad \text{in } \mathcal{Q}_{\bar{T}}(0), \\ \frac{\partial \hat{u}}{\partial \nu}(x, t) = \frac{\partial \hat{v}}{\partial \nu}(x, t) = 0 \quad \text{on } \Gamma_{\bar{T}}(0), \\ \hat{u}(y, 0) = \hat{u}_0(y), \hat{v}(y, 0) = \hat{v}_0(y) \quad \text{in } \bar{\Omega}_0, \end{array} \right. \quad (4.104)$$

where

$$\begin{aligned} F_1(\hat{u}, \hat{v}) &:= -\chi^2(t) f_1(\hat{u}, \hat{v}) - N \dot{\chi}(t) \chi(t) \hat{u}, \\ F_2(\hat{u}, \hat{v}) &:= \chi^2(t) f_2(\hat{u}, \hat{v}) - N \dot{\chi}(t) \chi(t) \hat{v}, \end{aligned}$$

with $\bar{T} = \varrho(T)$. we use that $t = \varrho(t)$ (without ambiguity).

4.4.2 Local existence and uniqueness of positive solutions

According to the conditions mentioned in the previous sub-section, the reaction function (F_1, F_2) is quasipositive, i.e. $F_1(0, \eta), F_2(\xi, 0) \geq 0$ for all $\xi, \eta \geq 0$. Hence, by supposing $\hat{u}_0, \hat{v}_0 \in L^\infty(\Omega_0)$, It is a well-known challenge to demonstrate the local existence, uniqueness, and nonnegativity of classical solution to the system (4.104) on $\Omega_0 \times [0, \bar{T}_{max})$ (cf. [46, 92]). Hence, we get the following result:

Theorem 4.4.1. We assume that $u_0, v_0 \in L^\infty(\Omega_0; \mathbb{R}_+)$ and (A1)-(A4) hold. Then, there exists a unique nonnegative classical solution of the system (4.96) on $\Omega_t \times [0, T_{max})$, where $0 < T_{max} \leq \infty$. Furthermore, if $T_{max} < \infty$, then

$$\lim_{t \rightarrow T_{max}} (\|u(\cdot, t)\|_{L^\infty(\Omega_t)} + \|v(\cdot, t)\|_{L^\infty(\Omega_t)}) = +\infty. \quad (4.105)$$

Thanks to the comparison principle, we get

$$0 \leq u(x, t) \leq \|u_0\|_\infty, \quad \forall (x, t) \in \Omega_t \times [0, T_{max}), \quad (4.106)$$

where $\|\cdot\|_\infty := \|\cdot\|_{L^\infty(\Omega_0; \mathbb{R}_+)}$.

4.4.3 Existence of global solutions

In order to prove the existence of global solutions to the system (4.96) we will derive an estimate for $\|F_2(\hat{u}, \hat{v})\|_{L^p(\Omega_0)}$ on $[0, \bar{T}_{max})$ for some $p > \frac{N}{2}$. For this aim, we suggest the following Lyapunov function (cf. [29]):

$$\mathcal{L}(t) = \int_{\Omega_0} \frac{e^{p\alpha(\hat{v}+1)^\beta}}{(K - \hat{u})^\mu} dy, \quad (4.107)$$

where $K, \alpha, \beta, \mu, p > 0$, such that

$$\begin{cases} \|u_0\|_\infty < K & \text{if } \ell = 0, \\ \|u_0\|_\infty < K < \frac{2\mu}{\alpha\beta N\ell} & \text{if } \ell > 0, \end{cases} \quad (4.108)$$

and

$$\beta \geq 1, \quad \mu \leq \frac{4d_1 d_2}{(d_1 - d_2)^2}, \quad (4.109)$$

with $d_1 \neq d_2$.

Theorem 4.4.2. Suppose that $u_0, v_0 \in L^\infty(\widehat{\Omega}_0)$ and the conditions (A1)-(A6) hold. Then, the solution of the main system (4.96) exists globally and it is uniformly bounded on $\Omega_t \times [0, \infty)$. The proof of the theorem follows immediately from the following results.

Proposition 4.4.1. The functional (4.107) satisfies the following differential inequality:

$$\frac{d}{dt} \mathcal{L}(t) \leq -C_1 \mathcal{L}(t) + C_2, \quad \forall t \in [0, \bar{T}^*], \quad \bar{T}^* \in (0, \bar{T}_{max}). \quad (4.110)$$

Where C_1 and C_2 are some positive constants.

Proof. It is similar to that found in the previous section. ■

Corollary 4.4.1. Under the assumptions (A1)-(A6) and $\hat{u}_0, \hat{v}_0 \in L^\infty(\Omega_0)$, the solution (\hat{u}, \hat{v}) of system (4.104) is uniformly bounded. Thus, the solution (\hat{u}, \hat{v}) exists globally.

Proof. It can be reached by following the same footsteps in the previous section. ■

4.4.4 Global stability of solutions

In this part, we prove the global stability of solution of the system (4.102) (thus, for the main system) by using the following candidate Lyapunov function:

$$\mathcal{V}(t) = \frac{1}{2} \int_{\Omega_0} [\varsigma \bar{u}^2 + 2\bar{u}\bar{v} + \bar{v}^2] dy, \quad (4.111)$$

where

$$\varsigma > \frac{(d_1 + d_2)^2}{4d_1d_2}. \quad (4.112)$$

We must have the following Lemma:

Lemma 4.4.1. Suppose that $(\bar{u}_0, \bar{v}_0) \in (C^2(\Omega_0) \cap C(\bar{\Omega}_0))^2$. Let (\bar{u}, \bar{v}) be a solution of system (4.102). Thus, there exist two positive constant $\nu \in (0, 1)$ and C^* , such that the following estimates hold:

$$\|\bar{u}(y, \cdot)\|_{C^{\frac{\nu}{2}+1}([1, \infty))} + \|\bar{v}(y, \cdot)\|_{C^{\frac{\nu}{2}+1}([1, \infty))} \leq C^*, \quad \forall y \in \bar{\Omega}_0, \quad (4.113)$$

and

$$\|\bar{u}(\cdot, t)\|_{C^{\nu+2}(\bar{\Omega}_0)} + \|\bar{v}(\cdot, t)\|_{C^{\nu+2}(\bar{\Omega}_0)} \leq C^*, \quad \forall t \geq 1. \quad (4.114)$$

Proof. Thanks to the parabolic-type L^p and Schauder estimates as well as embedding theorems (cf. [56, 62, 110, 111]) we can get the required results. ■

Theorem 4.4.3. Suppose that the assumptions (A1)-(A6) hold, in addition to

$$0 \leq \Psi(\eta) \leq 1, \quad \forall \eta \in \mathbb{R}_+,$$

and let $(\bar{u}_0, \bar{v}_0) \in \left(C^2(\Omega_0) \cap C(\bar{\Omega}_0)\right)^2$, we suppose also the evolution function χ is exponential. Hence, the trivial solution (i.e. $(0, 0)$) of system (4.102) is globally asymptotically stable in the following sense:

$$\lim_{t \rightarrow \infty} \|\bar{u}(\cdot, t)\|_\infty = \lim_{t \rightarrow \infty} \|\bar{v}(\cdot, t)\|_\infty = 0. \quad (4.115)$$

Proof. It is similar to that found in the previous section. ■

4.4.5 Examples and numerical experiments

We examine a specific case of system (4.96). To create the Figures, we employed numerical analysis as well as Matlab software. We have selected the parameters as follows: $T = 10000$, $(d_1, d_2) = (1, 3)$,

$$\left\{ \begin{array}{l} f(\xi, \eta) = \xi(1 + \eta^3) e^{\eta^2}, \\ g(\xi, \eta) = \xi e^{\eta^2}, \\ \Psi(\eta) = \frac{1}{1 + \eta^3}, \\ \phi(\xi) = \xi. \end{array} \right.$$

and $\chi(t) = e^{3 \times 10^{-4} t}$. We assume that the initial data are bounded and smooth:

$$\left\{ \begin{array}{l} u_0(y) = 1 + 0.09 \cos(7\pi y), \\ v_0(y) = 0.98 - 0.09 \sin(7\pi y). \end{array} \right.$$

Figures 4.9-4.10 represent the numerical solution $(u(x, t), v(x, t))$ of the main proposed system (4.96) in the cases of time-varying domain, they confirm the theoretical results (existence and uniform boundedness of solution), as well as, we observe that (u, v) do converge towards to the trivial solution $(0, 0)$.

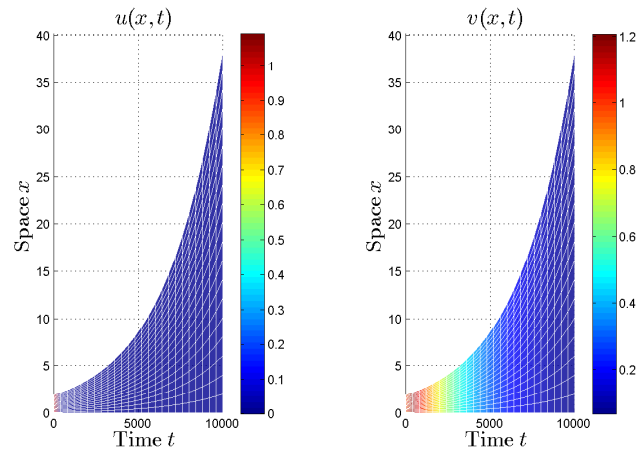


Figure 4.9: The numerical solution of the main proposed system (4.96) on growing domain $\Omega_t = (0, 2\chi(t))$ with $t \in [0, T]$, and subject to the proposed data.

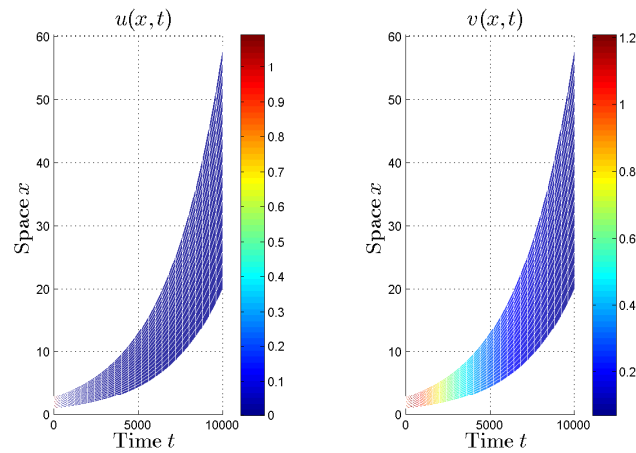


Figure 4.10: The numerical solution of the main proposed system (4.96) on growing domain $\Omega_t = (\chi(t), 3\chi(t))$ with $t \in [0, T]$, and subject to the proposed data.

CONCLUSION

The primary goal of this thesis is to investigate reaction-diffusion systems as a model for pattern formation. The main outcomes of this investigation can be divided into two categories. Firstly, we have analysed time-fractional reaction-diffusion systems as well as we proposed efficient numerical methods to solve such systems. Moreover, our analysis paved the way for a study of the Turing-Instability of time-fractional reaction-diffusion systems, these results give more dynamics in order to model biological pattern formation. Secondly, we discussed the open question about the global existence of solutions of activator-inhibitor reaction-diffusion systems and other system related, on the evolving domains, and we also came to identify the behavior of solutions for such systems under certain conditions, we used numerical analysis to support and confirm our results. Including evolving of spacial domain in partial differential equations during modelisation is an effective tool for deep understanding of phenomena in which the spatial domain is dependant on the time variable, especially in developmental biology.

During the preparation of this thesis we came across many new ideas that can be studied on reaction-diffusion systems, among the possible extensions of our work, we cite as example:

- Consider time-space fractional reaction-diffusion systems with various smooth nonlinearities and prove the global existence of solutions, as well as investigate behaviour of solutions.
- The question about global existence of reaction-diffusion systems with complex evolution of domains and general reaction terms is still open, the same for asymptotic behaviors of solutions for such systems.

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