DERIVATION OF FRACTIONAL-ORDER MODELS FROM A STOCHASTIC PROCESS

A thesis submitted for the degree of

Doctor of Philosophy

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Supervised by Professor Bruce Henry and Doctor Christopher Angstmann

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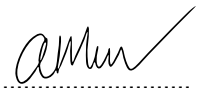
Signed 

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Fractional calculus has a long history, almost as old as calculus itself, dating back to the late seventeenth century. There has been a great deal of mathematical interest in this area by pure mathematicians but it is only in recent decades that the applications of fractional calculus have been systematically explored. The physical interest in fractional calculus is due to it's nonlocal nature which introduces a history dependence into the system.

Differential equations are the mainstay of mathematical models that describe and predict the evolution of systems in time. It is intuitive to replace some of the integer order time derivatives with fractional order time derivatives to provide a model that incorporates a history dependence. However, including fractional derivatives in this way can lead to problems in reconciling the dimensions of parameters in the systems. In this thesis we have developed a modelling approach, to include fractional derivatives and a history dependence, which is based on a well defined stochastic process. The resulting fractional order models and their parameters are well posed.

The thesis begins with a discussion of the history of fractional calculus, leading to the application to partial differential equations (PDEs), derived from continuous time random walks (CTRWs). We provide a brief overview of CTRWs and their role in deriving fractional order ordinary di↵erential equations (ODEs) and PDEs. Some of the fundamental tools of fractional calculus are introduced. A discrete time analogue of a CTRW is also introduced.

After the introductory material, the remainder of the thesis is a compilation of original published work that I have co-authored. This material is separated into 5 three parts. Part I, consisting of Chapters 2 - 7, features the derivation of fractional order ODE models and their discretisations. Part II, consisting of Chapters 8 - 10, is focused on the derivation of fractional PDE models. Part III, consisting of Chapters 11 - 12, presents novel numerical approaches for solving fractional-order ODEs and PDEs via piecewise approximations.
This thesis includes the results drawn from nine published papers produced over the course of my PhD candidature.

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Abstract

Fractional calculus has a long history, almost as old as calculus itself, dating back to the late seventeenth century. There has been a great deal of mathematical interest in this area by pure mathematicians but it is only in recent decades that the applications of fractional calculus have been systematically explored. The physical interest in fractional calculus is due to it's nonlocal nature which introduces a history dependence into the system.

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Arising Publications

Here is a list of publications arising during the course of my doctoral candidature. In all but the last article, authors are listed alphabetically. An asterisk denotes that I was the primary or joint primary co-author.

*C. N. Angstmann, A. M. Erickson, B. I. Henry, A. V. McGann, J. M. Murray, and J. A. Nichols. Fractional order compartment models. *SIAM J. Appl. Math.*, 77(2):430–446, 2017.

C. N. Angstmann, B. I. Henry, B. A. Jacobs, and A. V. McGann. Discretization of fractional differential equations by a piecewise constant approximation. *Math. Model. Nat. Pheno.*, 12(6):23–36, 2017.

*C. N. Angstmann, B. I. Henry, B. A. Jacobs, and A. V. McGann. Integrablization of time fractional PDEs. *Comput. Math. Appl.*, 73(6):1053–1062, 2017.

*C. N. Angstmann, B. I. Henry, B. A. Jacobs, and A. V. McGann. A time-fractional generalised advection equation from a stochastic process. *Chaos Solitons Fractals*, 102:175–183, 2017.

C. N. Angstmann, B. I. Henry, B. A. Jacobs, and A. V. McGann. An explicit numerical scheme for solving fractional order compartment models from the master equations of a stochastic process. *Commun. Nonlinear Sci. Numer. Simul.*, page In Press, 2019.

*C. N. Angstmann, B. I. Henry, and A. V. McGann. A fractional-order infectivity SIR model. *Phys. A*, 452:86–93, 2016.

*C. N. Angstmann, B. I. Henry, and A. V. McGann. A fractional order recovery SIR model from a stochastic process. *Bull. Math. Biol.*, 78(3):468–499, 2016.

*C. N. Angstmann, B. I. Henry, and A. V. McGann. A fractional-order infectivity and recovery SIR model. *Fractal Fract.*, 1(1):11, 2017.

*C. N. Angstmann, B. I. Henry, and A. V. McGann. Generalized fractional diffusion equations for subdiffusion in arbitrarily growing domains. *Phys. Rev. E*, 96(4):042153, 2017.

J. C. Walsh, C. N. Angstmann, A. V. McGann, B. I. Henry, I. G. Duggin, and P. M. G. Curmi Patterning of the MinD cell division protein in cells of arbitrary shape can be predicted using a heuristic dispersion relation. *AIMS Biophysics*, 3(1): 119-145, 2016.

Contents

Chapter 1

Introduction

Fractional calculus has a long history dating back to the origins of calculus in the late 1600s [121]. In the past few decades there has been renewed interest in fractional calculus due to modelling applications. Fractional calculus mathematical models are typically written as ordinary differential equations (ODEs) or partial differential equations (PDEs) with fractional derivatives. The incorporation of fractional derivatives introduces a history dependence into the model; the future state is dependent on all past states. These models have been applied to a variety of contexts; including anomalous diffusion [106], epidemiology [21], pharmacokinetics [144] and viscoelasticity [97].

In recent years it has become popular to investigate mathematical models with fractional derivatives included in an *ad hoc* fashion, by replacing standard derivatives with fractional derivatives. This direct derivative substitution introduces more parameters, e.g. the order of the derivatives, and thus can result in better fitting models or lead to interesting mathematical results. However from a modelling perspective replacing ordinary derivatives with fractional derivatives can lead to inconsistent model dimensions and thus the clear interpretation of parameters may be lost. This thesis provides a physically consistent method, using an underlying stochastic process, as a basis for deriving fractional equations. The method can be applied to both ODE and PDE systems and in this thesis it is applied to compartment models and diffusion processes on non-uniform domains.

1.1 Brief History

The origin of fractional calculus is generally dated back to a letter exchange between l'Hôpital and Leibniz in 1695 [86]. In their exchange, they consider the possibility of taking a derivative with order $\frac{1}{2}$. Whilst this provides an anecdotal and oft quoted introduction to the field, it was not until the 19th century that formal mathematical definitions of the fractional integral and derivative were formulated.

The first recorded use of fractional calculus occurred by Abel in 1823 [3, 4]. In order to solve the tautochrone problem, Abel introduces formulas which can be recognised as a fractional integral and derivative [122]. The properties of fractional derivatives are exploited in order to solve the problem. However, it was not until 1834 that the Riemann-Liouville fractional integral and derivative were formally defined by [91].

There has been increased attention in the fractional calculus arena over the past fifty years as the applications of fractional derivatives have become more apparent. This interest has occurred across multiple subfields. In particular the history dependence that fractional derivatives introduce were found to be useful in viscoelasticity. This was first noted by Caputo in 1967 [34] and explored in greater detail by Mainardi [95, 96]. Mainardi makes use of the fractional diffusion considered by Wyss [154], which is defined by replacing the standard temporal derivative with a time-fractional derivative.

The applications of fractional calculus have also been seen in the development of diffusion equations from the limit of the continuous time random walk (CTRW) [111, 133]. If the CTRW has a history dependence the resulting diffusion equations may include time-fractional derivatives [67, 35, 28, 106]. Fractional diffusion equations obtained in this manner model anomalous diffusion in which the mean squared displacement does not scale linearly. CTRWs have been generalised in various ways to model fractional diffusion with reactions [63, 142], forces [60, 61], trapping [7], and on non-uniform, see Chapter 9, and on growing domains [85, 23].

The remainder of the first chapter will provide a more detailed introduction and background to the areas of mathematics required in deriving fractional ODE and PDE models from underlying stochastic processes. This will include CTRWs in Section 1.2, anomalous diffusion in Section 1.3, compartment models in Section 1.4 and fractional derivatives and their properties in Section 1.5. The related discretisations and numerical schemes for fractional models are introduced in Section 1.7.

1.2 Continuous Time Random Walks

The random walk was introduced by; Bachelier in his PhD thesis [25], by Pearson in a problem posed in Nature [116], and by Einstein in his consideration of Brownian motion [46]. Einstein showed that the probability density function describing the position of a random walk was governed by the diffusion equation. In general terms this demonstrates a connection between stochastic processes and PDEs. In the past few decades this connection has been greatly expanded through the consideration of CTRWs and their limit processes.

The CTRW was originally considered by Montroll and Weiss in 1965 [111] and further developed by Scher and Lax [133]. This approach was further generalised over the following decades [125, 148, 137, 112, 79]. Partial differential equations can be derived by taking an appropriate diffusion limit of the master equation of a CTRW. An advantage of constructing PDEs from a CTRW is that the model parameters can be understood easily as physical processes and the CTRW describes the dynamic process at a mesoscopic level.

The CTRW is set up by considering the governing dynamics of an individual walker on a lattice and extending this consideration to an ensemble of walkers. In the CTRW each walker waits at a site, x', for an amount of time drawn from a waiting time density, $\psi(t)$, before jumping to a new site, x, governed by the jump density $\lambda(x, x', t)$. Let us now consider an ensemble of walkers, where each walker is governed by a common jump density, $\lambda(x, x', t)$, and a common waiting time density, $\psi(t)$. The expected concentration of walkers at any given site can now be expressed.

By taking the limit in which the distance between the lattice sites goes to zero, the dynamics of the walkers can be considered on a spatial continuum. The diffusion limit requires both the lattice spacing to go to zero and the characteristic time-scale to go to zero. This needs to be done carefully to avoid singularities and this will be discussed further in subsequent sections of this thesis.

If the central limit theorem holds for the stochastic process of the CTRWs then the walkers will be undergoing Brownian motion [55, 32, 106] and the dynamics of their concentration will be described by a standard diffusion equation. Standard diffusion is characterised by the mean squared displacement growing proportionally with time [116], i.e.,

$$\langle X^2(t)\rangle \sim t. \tag{1.1}$$

The central limit theorem does not hold for all choices of jump densities or waiting time densities. In particular if the jump or waiting time density has a power-law tail, for example a Pareto or Mittag-Leffler density, the central limit theorem does not hold. The work in this thesis focuses on power-law waiting time densities. As the first moment of power-law distributions diverges, the standard central limit theorem does not appy to describe the resulting dynamics of the walkers. However the Lévy-Gnedenko generalised central limit theorem [57, 88] can be applied and making use of the properties of geometrically stable distributions, a power-law waiting time produces anomalous diffusion. The diffusion limit of the master equations for CTRWs with power-law waiting times can be expressed with time-fractional derivatives. The mean squared displacement calculated from these fractional diffusion equations has anomalous scaling, i.e.,

$$\langle X^2(t)\rangle \sim t^\alpha, \tag{1.2}$$

for $\alpha \neq 1$. This result, commonly referred to as anomalous diffusion, has been experimentally observed across a variety of settings, so much so that it has been

noted that "*Anomalous is ubiquitous*" [52] and has lead to increasing interest in the mathematical nature of anomalous diffusion.

1.3 Subdiffusion

The size of α in Eq. (1.2) quantifies the anomalous diffusion. In particular this thesis focuses on subdiffusion, classified by $0 < \alpha < 1$. Subdiffusion has been commonly observed in biological systems with traps and obstacles [131, 45, 151]. It has also been observed in the diffusion of molecules in spiny nerve cells [129], diffusion across potassium channels in membranes [99, 150], and diffusion of HIV virions in cervical mucous [138]. Subdiffusion is also present in other physical systems such as cosmic rays [136], porous media [87], and volcanic earthquakes [2].

The equation for subdiffusion is a generalisation of the standard diffusion equation. This equation can be expressed with a fractional derivative [28],

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left({}_0\mathcal{D}_t^{1-\alpha}\left(\rho(x,t)\right)\right), \tag{1.3}$$

and as $\alpha \to 1$ the equation limits to the standard diffusion equation. The notable difference between the subdiffusion equation and the standard diffusion equation, is the presence of the Riemann-Liouville fractional derivative, ${}_0\mathcal{D}_t^{1-\alpha}\left(\rho(x,t)\right)$. The definition for this and other fractional derivatives are presented in Section 1.5.

Before the stochastic derivation of the subdiffusion equation, Wyss replaced the time derivative of the standard diffusion equation with a fractional derivative [154] and analysed it's mathematical properties. This equation was found to be useful in modelling viscoelasticity by Mainardi [95]. Hilfer and Anton derived the master equation using the CTRW framework [67], which after taking a diffusion limit, results in the subdiffusion equation. In doing so Hilfer and Anton considered a Mittag-Leffler waiting time density [121]. Building on [79], Compte took the diffusion limit of this master equation [35], deriving an equation for subdiffusion which was identical to Wyss' equation.

The equation for subdiffusion with forces and/or reactions was subsequently derived from the CTRW framework. The incorporation of subdiffusion has proven non-trivial in these extensions. In a standard Fokker-Planck equation or reaction-diffusion equation the diffusion is independent of either the forces or reactions respectively. However, one of the notable results from the derivation of subdiffusive equations with forces or reactions is that the diffusion can affect the forcing or reactions. Subdiffusion with forcing was introduced by implementing a power-law waiting time density and a time biased jump length density in the CTRW, resulting in a fractional Fokker-Planck equation [105, 104, 28, 106]. Space dependent forcing and time dependent forcing has also been considered in this context [142, 61, 11]. An equation with fractional-advection, with no diffusion, has also been derived from the CTRW framework [18].

By introducing a source term along with power-law waiting times, reactions were able to be introduced, giving rise to fractional reaction-diffusion equations [63, 62, 143, 83, 53, 1, 158]. More recently, the equation for subdifffusion with both forcing and reaction was systematically derived [7]. These fractional equations have been derived outside of the CTRW framework as well [152, 93, 141].

Another area of interest has been in deriving PDEs on a growing domain. Over the past two decades, equations for diffusion, forcing and reactions have been derived on a growing domain [36, 113, 37, 153]. These equations have been generalised to account for more complex forcing and non-uniform growth [26, 155, 140, 157]. A natural extension has been to consider subdiffusion on a growing domain [23, 85].

My contribution to this field has been the derivation of the fractional-advection equation without diffusion, which makes up Chapter 8, subdiffusion on a geometrically spaced lattice, in Chapter 9 and subdiffusion on a growing domain, Chapter 10.

1.4 Compartment Models

In addition to considering the derivation of fractional-order PDEs, this thesis also considers the derivation of fractional-order ODE models. In particular, this thesis contains the derivations for epidemiological models containing fractional derivatives, as well as the derivation for a general fractional-order compartment model. A compartment model is a mathematical model which describes the dynamics of entities moving between different compartments. Typically the compartments are assumed to be homogeneous, i.e. all elements in the compartment are assumed to have the same probabilities of leaving the compartment. These models are typically represented by a set of coupled ODEs with time the independent variable. The dependent variable may represent numbers of entities or concentrations of entities.

These models have been applied to a range of contexts, including epidemiology [73, 64], pharmacokinetics [144] and economics [70, 147]. The particular quantities of interest vary between applications. For example in a compartment model for epidemiology, the compartments represent states in which individuals are susceptible, infected, or removed from the infection, commonly known as an SIR model [73]. While in pharmacokinetic compartment models, the compartments may represent the concentration of particular drugs in various organs in a person's body.

If the transition between compartments are Markovian, i.e., they do not depend on the 'age' of the system, the dynamics can be captured by standard ODE models. In such models, the time when 'particles' leave a compartment is not dependent on how long they have spent in the compartment. If the behaviour of the particles is dependent on how long they have been in a compartment, then the mathematical formulation of the compartment model can no longer be captured by autonomous ODEs. There are many examples of systems in which the length of time particles have spent in a given state, represented as a compartment, will affect their subsequent behaviour. Such systems are said to have a history dependence. There are a variety of methods of capturing the system's history dependence, including the use

of non-local operators such as integro-differential terms and fractional derivatives [74, 75, 65, 44, 43, 59, 21, 20, 14, 130, 144]. The growing interest in fractional ODE models can, in part, be attributed to the popularity of fractional derivatives in PDEs [42].

The original epidemiological compartment model was introduced by Kermack and McKendrick [73]. They proposed a three compartment model, commonly referred to as the SIR model. The model splits the population into three classes, those susceptible (S), infected (I) and recovered (or removed) (R) from the infection. In this model individuals begin susceptible to the infection, through interaction with an infected individual they may become infected and moved to the infected class, before finally recovering from the disease and developing immunity to the infection. This can be described by the ODE system,

$$\frac{dS}{dt} = \lambda - \beta SI - \gamma S, \tag{1.4}$$

$$\frac{dI}{dt} = \beta SI - \omega I - \gamma I, \tag{1.5}$$

$$\frac{dR}{dt} = \omega I - \gamma R, \tag{1.6}$$

in which λ and γ are the birth and death rates respectively. In these equations it is assumed that birth and death rates are the same for all compartments. Susceptible individuals become infected after contact with an infected individual with probability β and $\frac{1}{\omega}$ is the expected infected time before individuals recover. All individuals are subject to the same recovery rate regardless of how long they have been infected.

Many variations of the SIR model have been proposed [64], typically through the introduction of a new state, resulting in an additional compartment, or creating a new path between states. Some SIR extensions include; the possibility for waning immunity after an individual has recovered from an infection; and having an incubation time before infected individuals become infectious. These extensions produce autonomous, coupled ODE systems. The limitations of autonomous ODE models

can be seen in epidemiological applications when considering a chronic infection. If a disease is known to be chronic, the longer an individual has been infected, the less likely they are to recover [126]. This property cannot be captured by a standard ODE epidemic model.

The earliest non-autonomous SIR model is the age-structured SIR model introduced by Kermack and McKendrick in 1932 [74], in the form of integro-differential equations. The age-structuring of this model refers to the 'age' of the infection. Given that the length of time that an individual is infected will affect the dynamics, the model incorporates a history dependence. In such a model individuals who have been infected for different amounts of time may be subject to different recovery probabilities. This model reduces to the standard Eqs. (1.4), (1.5) and (1.6) when individuals have the same chance of recovering, regardless of how long they have been infected.

A more recent approach to incorporating history dependence into compartment models is to consider a fractional-order compartment model. We have derived fractional SIR models by allowing for the inclusion of memory effects on the infectivity or recovery of the infection [21, 20, 22]. Fractional pharmacokinetic models allow for the modelling of drugs which lead to long term accumulation [42, 44, 43, 59]. The inclusion of memory effects through fractional derivatives in economic models has also been considered [145, 146]. We have also derived a general fractional order compartment model that can be adopted to different applications [14].

Our approach in deriving fractional order compartment models has been to consider an underlying stochastic process, representing a CTRW between compartments [21, 20, 14, 22, 130]. This is analogous to the derivation of PDEs from CTRWs, discussed in Section 1.2. Using a CTRW, a compartment model can be derived with an arbitrary survival probability density. Choosing a memoryless survival density will produce a standard compartment model, while choosing a heavy-tailed power-law density leads to a fractional-order compartment model. This type of derivation is used to produce different sorts of fractional order SIR models including; a fractional

recovery SIR model in Chapter 2 [21]; a fractional infectivity SIR model in Chapter 4 [20]; a fractional infectivity with fractional recovery SIR model in Chapter 5 [22]; and a general fractional order compartment model in Chapter 3 [14].

1.5 Introductory Fractional Calculus

A cursory understanding of fractional calculus, specifically fractional derivatives, is fundamental to this thesis. Here I present a set of definitions and properties of the necessary fractional derivatives to understand the fractional models derived throughout this thesis.

The canonical definition for the fractional integral, also known as the Riemann-Liouville integral, is given by,

$$ {}_0\mathcal{D}_t^{-\alpha} f(x,t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(x,\tau) d\tau, \tag{1.7} $$

for $\alpha \in \mathbb{R}^+$. This definition is a generalisation of the Cauchy n-fold integral, extending $n \in \mathbb{N}$ to allow for all positive reals.

Unlike integer order derivatives, there are multiple, contradictory definitions for fractional derivatives [115, 128, 121, 89]. Riemann-Liouville, Caputo and Grünwald-Letnikov fractional derivatives will feature throughout this thesis. These fractional derivatives are introduced in this section along with the generalised fractional derivative and Riesz space fractional derivative. The Riemann-Liouville fractional derivative, with order $\alpha \in \mathbb{R}^+$, is given by taking an integer order derivative of the Riemann-Liouville fractional integral [115], defined as,

$$ {}_{RL}\mathcal{D}_{0,t}^{\alpha} f(x,t) = \frac{\partial^m}{\partial t^m} {}_0\mathcal{D}_t^{-(m-\alpha)} f(x,t) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial t^m} \int_0^t (t-\tau)^{m-\alpha-1} f(x,\tau) d\tau, \tag{1.8} $$

with $m-1 \leq \alpha < m$ and $m \in \mathbb{N}$. The fractional derivative can be seen as a generalisation of an integer order derivative explicitly in Laplace space. The Laplace

transform, from t to s, of the fractional derivative is,

$$\mathcal{L}\left\{ {}_{RL}\mathcal{D}^{\alpha}_{0,t} f(x,t)\right\} = s^{\alpha}\mathcal{L}\{f(x,t)\} - \sum_{k=0}^{m-1} s^{k}\, {}_{0}\mathcal{D}^{\alpha-k-1}_{t} f(x,t)\Big|_{t=0}. \tag{1.9}$$

However, the initial conditions required for this Laplace transform are in the form of a fractional integral over the function's history [66]. The Caputo fractional derivative was proposed [34] to enable standard initial conditions. The Caputo fractional derivative, with order $\alpha \in \mathbb{R}^{+}$ is defined as,

$${}_{C}\mathcal{D}^{\alpha}_{0,t} f(x,t) = {}_{0}\mathcal{D}^{-(m-\alpha)}_{t} \frac{\partial^{m}}{\partial t^{m}} f(x,t) = \frac{1}{\Gamma(\alpha)} \int_{0}^{t} (t-\tau)^{\alpha-1} \frac{\partial^{m}}{\partial \tau^{m}} f(x,\tau) d\tau, \tag{1.10}$$

with $m-1 \leq \alpha < m$. The Laplace transform of the Caputo fractional derivative is,

$$\mathcal{L}\{ {}_{C}\mathcal{D}^{\alpha}_{0,t} f(x,t)\} = s^{\alpha}\mathcal{L}\{f(x,t)\} - \sum_{k=0}^{m-1} s^{\alpha-k-1} \frac{\partial^{k} f(x,t)}{\partial t^{k}}\bigg|_{t=0}, \tag{1.11}$$

for $m-1 \leq \alpha < m$, for $m \in \mathbb{N}$. The initial conditions here involve integer order derivatives at a point, and the Caputo derivative of a constant is zero. Some researchers cite these as reasons to use the Caputo derivative rather than the Riemann-Liouville derivatives [34]. However a disadvantage of the Caputo derivative is that it does not limit to an ordinary derivative in the limit as $\alpha \to (m-1)^{+}$ [89]. Moreover, despite the differences between the Riemann-Liouville and Caputo derivatives, an elementary relationship exists between the two derivatives,

$${}_{RL}\mathcal{D}^{\alpha}_{0,t} f(x,t) = {}_{C}\mathcal{D}^{\alpha}_{0,t} f(x,t) + \sum_{k=0}^{m-1} \frac{t^{k-\alpha}}{\Gamma(1-\alpha+k)} \frac{\partial^{k} f(x,t)}{\partial t^{k}}\bigg|_{t=0}. \tag{1.12}$$

The two derivatives are equivalent if,

$$\frac{\partial^{k} f(x,t)}{\partial t^{k}}\bigg|_{t=0} = 0, \tag{1.13}$$

for all $k = 0, 1, ..., m-1$.

The third fractional derivative, that is widely used in this thesis, is the Grünwald-Letnikov derivative, defined by,

$$ {}_{GL}\mathcal{D}^{\alpha}_{0,t} f(x,t) = \lim_{h\to 0, nh=t} h^{-\alpha} \sum_{k=0}^{n} (-1)^k \binom{p}{k} f(x, t-kh). \tag{1.14} $$

This derivative is equivalent to the Riemann-Liouville derivative for functions $f(x,t)$, which are sufficiently smooth around $t = 0$. This equivalence can be seen more clearly in the alternate definition for the Grünwald-Letnikov derivative [89],

$$ {}_{GL}\mathcal{D}^{\alpha}_{0,t} f(x,t) = \sum_{k=0}^{m-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} \frac{\partial^k f(x,t)}{\partial t^k}\bigg|_{t=0} + \frac{1}{\Gamma(m-\alpha)} \int_0^t (t-\tau)^{m-\alpha-1} \frac{\partial^m f(x,t)}{\partial t^m} d\tau. \tag{1.15} $$

The Grünwald-Letnikov derivative is included here as it's limit form provides a basis for numerical schemes for fractional-order differential equations [159]. This is done by considering a small enough h and taking a finite sum approximation.

The generalised fractional derivative is typically defined through it's Laplace transform,

$$ \mathcal{L}\{ {}_{G}\mathcal{D}^{\alpha}_{0,t} f(x,t)\} = s^{\alpha} \mathcal{L}\{f(x,t)\}, \tag{1.16} $$

which is equivalent to the Riemann-Liouville derivative, Eq. (1.8), when $0 \leq \alpha < 1$ and $x(t)$ is sufficiently regular around $t = 0$. A more formal definition for the generalised fractional derivative is provided in [89].

Another common fractional derivative is the Riesz fractional derivative [124]. This derivative is typically derived through it's Fourier transform [30] rather than it's Laplace transform,

$$ \mathcal{F}\{R^{\alpha}_{x} f(x,t)\} = -|\omega|^{\alpha} F(\omega, t), \tag{1.17} $$

where $F(\omega, t)$ is the Fourier transform of $f(x,t)$. This derivative is used commonly in 'space' fractional systems, however this is beyond the scope of this thesis and will not be discussed further.

I have presented the partial derivative form of the fractional derivatives. Originally these derivatives were proposed as total derivatives, however it has become common to use the same notation for fractional derivatives, regardless of whether they are being taken of a function with one or more variables. Hence when we consider ODE systems, we will use the same notation as that of the PDE systems.

While all the fractional derivatives presented above are valid for $\alpha \in \mathbb{R}^+$, from this point forward I limit my discussion of these derivatives to the $0 \leq \alpha < 1$ case. This is due to their association with power-law, heavy tailed distributions, [67] trapping [7, 21] and subdiffusion [106] processes. It is with these applications in mind that I have incorporated fractional derivatives into the ODE [21, 20, 14, 22, 19] and PDE [17, 23] models.

I have constrained this very brief introduction on fractional calculus to the definitions and properties that I make use of in the later chapters of this thesis. For a more thorough introduction into fractional calculus please see [115, 127, 107, 121].

1.6 Generalized Caputo Models with Unknown Derivation Methods

The major motivation for Part I of this thesis is to introduce and implement a systematic approach for including fractional differential operators into ODE models. Our approach, based on underlying stochastic process with history dependence, leads to the formal introduction of fractional differential operators. This avoids physical problems that arise when integer order derivatives are simply replaced with fractional derivatives. To focus on these problems, consider the following *ad hoc* fractional SIR model:

$$\frac{d^{\alpha_1} S}{dt^{\alpha_1}} = \lambda - \beta SI - \gamma S, \tag{1.18}$$

$$\frac{d^{\alpha_2} I}{dt^{\alpha_2}} = \beta SI - \omega I - \gamma I, \tag{1.19}$$

$$\frac{d^{\alpha_3} R}{dt^{\alpha_3}} = \omega I - \gamma R. \tag{1.20}$$

An assumption of the SIR model is that the flux out of one compartment matches the flux into a corresponding one i.e. the number of individuals leaving the susceptible compartment, due to becoming infected, will match the number of incoming infected individuals. The flux-balance is violated when $\alpha_1 \neq \alpha_2$. A similar violation occurs when $\alpha_2 \neq \alpha_3$, resulting in a flux-balance violation of the number of individuals recovering from the infection.

If we let $[a]$ denote the dimensions of the parameter a, and carry out a simple dimensional analysis of this system then: from Eq. (1.18) the dimensions of the parameters are $[\lambda] = \text{time}^{-\alpha_1}$, $[\beta] = \text{time}^{-\alpha_1}$, $[\gamma] = \text{time}^{-\alpha_1}$, from Eq. (1.19) $[\beta] = \text{time}^{-\alpha_2}$, $[\omega] = \text{time}^{-\alpha_2}$, $[\gamma] = \text{time}^{-\alpha_2}$ and from Eq. (1.20) $[\omega] = \text{time}^{-\alpha_3}$, $[\gamma] = \text{time}^{-\alpha_3}$. This analysis highlights potential inconsistent dimensions of the model parameters. Similar issues arising from *ad hoc* fractional models were noted by Dokoumetzidis, Magin and Macheras, in the context of fractional pharmacokinetic models [43, 44].

To reconcile both the flux balance and dimensional issues, we require $\alpha_1 = \alpha_2$ and $\alpha_2 = \alpha_3$; i.e., $\alpha = \alpha_1 = \alpha_2 = \alpha_3$. If we now add Eqs. (1.18), (1.19) and (1.20) and define the total population, N, as $N = S + I + R$ then,

$$\frac{d^\alpha N}{dt^\alpha} = \lambda - \gamma N. \tag{1.21}$$

If the birth rate is equal to the death rate then $\lambda - \gamma N = 0$, which requires $\frac{d^\alpha N}{dt^\alpha} = 0$. If $\frac{d^\alpha}{dt^\alpha}$ is a Riemann-Liouville fractional derivative, this would imply $N = 0$. If $\frac{d^\alpha}{dt^\alpha}$ is a Caputo fractional derivative this particular issue is avoided. The resulting system,

$$\frac{d^\alpha S}{dt^\alpha} = \lambda - \beta SI - \gamma S, \tag{1.22}$$

$$\frac{d^\alpha I}{dt^\alpha} = \beta SI - \omega I - \gamma I, \tag{1.23}$$

$$\frac{d^\alpha R}{dt^\alpha} = \omega I - \gamma R, \tag{1.24}$$

where $\frac{d^\alpha}{dt^\alpha}$ is a Caputo fractional derivative is an SIR model with a history dependence but this is a very restricted generalisation and there is no obvious physical mechanism for the fractional derivative. In an SIR model with integer order deriviatives, the parameters have a clear physical interpretation and can be easily observed, i.e. λ represents the number of births per year. However in the fractional model governed by Eqs. (1.22), (1.23) and (1.24), the physical interpretation of the parameters is less clear, for example λ represents the number of births per year to the $-\alpha$. Our systematic approach for the incorporation of fractional derivatives, as outlined in Part I, resolves the above issues.

1.7 Discretisation of Fractional-Order Equations

The use of fractional derivatives within models can lead to difficulties in finding exact algebraic solutions. Many numerical methods have been proposed to numerically solve fractional ODEs [41, 156, 76, 120, 59, 161, 39, 16]. However the history dependence of fractional derivatives can make stable numerical methods complex to implement [19]. The approach considered throughout this thesis, to numerically deal with fractional-order ODEs, is to derive a corresponding discrete time random walk (DTRW) master equation. This DTRW is derived such that it limits to the CTRW when the length of the time steps approaches zero. These master equations can then be used as the basis for a stable numerical scheme. Furthermore, the equivalence of the Riemann-Liouville and Grünwald-Letnikov fractional derivatives [121] can be exploited in producing a discretisation. The Grünwald-Letnikov fractional derivative allows the Riemann-Liouville fractional derivative, used in our fractional-order ODEs, to be expressed as an infinite sum, Eq. (1.15), which can be truncated for a numerical scheme. This approach is considered for the discretisation of the fractional recovery SIR model in Chapter 6 and for a general fractional-order compartment model in Chapter 7.

1.8 Fractional-order Models

The focus of this thesis is the derivation of stochastically consistent fractional-order equations. The thesis is organised as follows. Part I, consisting of Chapters 2 - 7, focuses on the derivation of fractional order ODE models and their discretisations. This includes; derivation of an SIR model with a fractional recovery term; a derivation for a general multi-compartment system, where each compartment can have a multiple Markovian leaving terms and a single fractional leaving term; a derivation of a fractional infectivity SIR model; derivation of a fractional infectivity and fractional recovery SIR model; a discretisation of the fractional recovery SIR model; and a discretisation for general fractional compartment models.

Part II, consisting of Chapters 8 - 10, is concerned with the derivation of fractional PDE models. This includes; derivation of a fractional advection equation without diffusion; derivation for a time-fractional geometric Brownian motion equation; and derivation for the governing equation for anomalous diffusion on a growing domain.

Part III, consisting of Chapters 11 - 12, describes a novel numerical approach for solving fractional-order ODEs and PDEs via piecewise approximations.

Table 1.1 presents some of the fundamental equations derived throughout Parts I and II of this thesis.

Type	Example	Chapter
frODEs	$\frac{dI}{dt} = \omega S(t)I(t) - \gamma I(t) - \mu\theta(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right)$	2
	$\frac{d\rho_k}{dt} = q_k^+(t) - \omega_k(t)\rho_k(t) - \tau_k^{-\alpha_k}\Theta_k(t,0)\,{}_0\mathcal{D}_t^{1-\alpha_k}\left(\frac{\rho_k(t)}{\Theta_k(t,0)}\right)$	3
	$\frac{dI}{dt} = \omega(t)S(t)\Phi(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\Phi(t,0)}\right) - \mu(t)I(t) - \gamma(t)I(t)$	4
	$\frac{dI(t)}{dt} = \frac{\omega(t)S(t)\theta(t,0)}{\tau^\beta}\,{}_0\mathcal{D}_t^{1-\beta}\left(\frac{I(t)}{\theta(t,0)}\right) - \frac{\theta(t,0)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma(t)I(t)$	5
frPDEs	$\frac{\partial\rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(v(x,t)\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right)$	8
	$\frac{\partial S(x,t)}{\partial t} = D_\alpha\frac{\partial}{\partial x}\left(x^2\frac{\partial}{\partial x}\,{}_0\mathcal{D}_t^{1-\alpha}S(x,t) - \beta x^2F(x)\,{}_0\mathcal{D}_t^{1-\alpha}S(x,t)\right)$	9
	$\frac{\partial\rho(y,t)}{\partial t} = D_\alpha\frac{\partial^2}{\partial y^2}\left(e^{-rt}\,{}_0^g\mathcal{C}_t^{1-\alpha}\left(\rho(y,t)e^{rt}\right)\right) - ry\frac{\partial\rho(y,t)}{\partial y} - r\rho(y,t)$	10

Table 1.1: Some Fundamental Equations Derived in this Thesis

Part I

Fractional-Order ODE Models

Chapter 2

Fractional Recovery SIR

2.1 Introduction

This Chapter is based on the publication [21]. We derive a fractional recovery SIR model from an underlying physical stochastic process. We consider a variation of an SIR model where recovery from the disease is dependent on the time since infection. The model is derived from a directed CTRW through the SIR compartments, with the time in the infectious compartment drawn from a waiting time probability density. We show that, in the case of a power-law tailed waiting time density, the governing equations become a set of fractional-order differential equations. The expected recovery time diverges in a power-law waiting time density and this leads to chronic infection in the fractional recovery SIR model. As the fractional-order derivative operates on the recovery we refer to this as the fractional recovery SIR model. There have been several studies of semi-Markovian epidemic models in the recent literature [72, 109] that are related to the approach presented here, but they are not formulated as coupled integro-differential equations.

In Section 2.2 we derive an SIR model with an arbitrary waiting time before transitioning from the infectious compartment to the recovered compartment. This general model is shown to be consistent with the structured formulation of Kermack and McKendrick [74, 75]. We also derive an integral equation representation of the model and show that it reduces to the integral equations presented by Hethcote and Tudor [65] when the parameters are constants. In Section 2.3 we show that in

the case of a power-law waiting time distribution in the infectious compartment we obtain fractional-order derivatives in the model and we present the governing equations for the fractional recovery SIR model. Chapter 6 contains the discretisation and numerical scheme for the model derived in this Chapter.

2.2 SIR as a Continuous Time Random Walk

An underlying assumption in the simplest SIR models is that the transition of an individual through each of the compartments is independent of the amount of time since the individual entered the compartment. This assumption is mathematically equivalent to assuming that the time spent in each compartment is exponentially distributed. This is a very restrictive assumption with no a priori reason for it to hold. In some diseases with the potential for chronic infection, such as human papillomavirus (HPV), there is evidence of power-law tails in the distribution of infected times [126]. We have incorporated an arbitrary time in the infected compartment in our derivation of a generalised SIR model below by way of a CTRW [111, 133].

In this Chapter we derive an SIR model with births and deaths. This derivation may be adapted to any compartment model where the transition out of a compartment is dependent on the length of time since entering the compartment. This generalisation is presented in Chapter 3.

In the standard manner, we separate the population into three compartments, Susceptible (S), Infectious (I), and Recovered (R) [64]. The population is composed of individuals who are born into the S compartment and undergo a directed CTRW on the S, I, and R, compartments until they die and are removed from consideration. As in the standard model, individuals may only move from the S compartment to the I compartment and then to the R compartment. The transition to the I compartment occurs when an individual becomes infected and the transition to the R compartment occurs when an individual recovers from the infection. The derivation of fractional diffusion equations [67, 106], fractional reaction diffusion equations [62, 143, 53], fractional Fokker-Planck equations [28, 142, 61] and fractional chemotaxis diffusion

equations [82, 54] from CTRWs has been well studied and provides clear physical motivation for each of these systems. Our derivation of the evolution equations for the SIR model and fractional SIR model from a stochastic CTRW process with reactions is similar to the derivation of the fractional Fokker-Planck equation with reactions [7] and the derivation of the master equations for CTRWs with reactions on networks [8].

Consider an individual who is infectious. The probability that they will infect a susceptible person in the time t to $t+\delta t$ is assumed to be a product of the probability that the infectious person will encounter a susceptible and the probability that an encounter with a susceptible will result in an infection. Without loss of generality we can express the probability that an encounter with a susceptible will result in infection by $\omega(t)\delta t + o(\delta t)$, identifying $\omega(t)$ as the rate of becoming infected per time interval δt. Given that there are $S(t)$ susceptible people at time t, this implies that the probability of an infected individual creating a new infected individual in the time interval t to $t + \delta t$ is $\omega(t)S(t)\delta t + o(\delta t)$. We represent the number of individuals entering the infected state at time t, i.e. the flux, by $q^+(I,t)$, which can be recursively constructed from the flux at earlier times. Explicitly we have

$$q^+(I,t) = \int_{-\infty}^{t} \omega(t)S(t)\Phi(t,t')q^+(I,t')dt', \tag{2.1}$$

where $\Phi(t,t')$ is the probability that an infected individual has survived in the infected state until time t given that they entered the state at time t'. Let $i(-t',0)$ be the number of individuals who became infected at time $t' < 0$ and who are still infected at time 0, hence,

$$q^+(I,t') = \frac{i(-t',0)}{\Phi(0,t')}, \quad t' < 0. \tag{2.2}$$

We can then write Eq. (2.1) for $t \geq 0$ as,

$$q^+(I,t) = \int_0^t \omega(t)S(t)\Phi(t,t')q^+(I,t')dt' + \int_{-\infty}^0 \omega(t)S(t)\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt'. \quad (2.3)$$

For an individual to be in the infected compartment at time t they must have become infected at time t or at some prior time t' and remained in the compartment until t. The number infected at time t can therefore be found from the flux, and the survival probability, as follows,

$$I(t) = I_0(t) + \int_0^t \Phi(t,t')q^+(I,t')dt'. \quad (2.4)$$

Here we have defined the function,

$$I_0(t) = \int_{-\infty}^0 \frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt'. \quad (2.5)$$

We assume that there are two possible ways in which an individual can move from the infectious compartment; they can either recover from the disease and move to the R compartment, or they can die and be removed from consideration. If these two possibilities are independent we may write,

$$\Phi(t,t') = \phi(t-t')\theta(t,t') \quad (2.6)$$

where $\phi(t-t')$ is the probability of surviving the jump transition to the R compartment from time t' to time t, and $\theta(t,t')$ is the probability of surviving death from time t' until time t. If we have a time dependent death rate such that the probability of death occurring in the interval t to $t+\delta t$ is $\gamma(t)\delta t + o(\delta t)$, then the death survival can be written as,

$$\theta(t,t') = e^{-\int_{t'}^t \gamma(s)ds}. \quad (2.7)$$

The rate of change of the population in the infectious compartment can be found by differentiating Eq. (2.4) to get,

$$\begin{aligned}\frac{dI(t)}{dt} &= q^+(I,t) - \int_0^t \psi(t-t')\theta(t,t')q^+(I,t')dt' - \gamma(t)\int_0^t \phi(t-t')\theta(t,t')q^+(I,t')dt' + \frac{dI_0(t)}{dt} \\ &= q^+(I,t) - \int_0^t \psi(t-t')\theta(t,t')q^+(I,t')dt' - \gamma(t)I(t) + \theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right).\end{aligned} \tag{2.8}$$

Here we have used the fact that, $\phi(0) = 1$, and that the derivative of the jump survival function, $\phi(t)$, is a waiting time probability density function, here denoted $\psi(t)$, i.e.,

$$\frac{d\phi(t)}{dt} = -\psi(t). \tag{2.9}$$

Substituting Eq. (2.3) into Eq. (2.8) gives,

$$\begin{aligned}\frac{dI(t)}{dt} =& \omega(t)S(t)\left(\int_0^t \phi(t-t')\theta(t,t')q^+(I,t')dt' + I_0(t)\right) \\ &- \int_0^t \psi(t-t')\theta(t,t')q^+(I,t')dt' - \gamma(t)I(t) + \theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right).\end{aligned} \tag{2.10}$$

In order to obtain a generalised master equation we need to express the right hand side of this equation in terms of $I(t)$. We first use the definition of $I(t)$ in Eq. (2.4), to write,

$$\frac{dI(t)}{dt} = \omega(t)S(t)I(t) - \int_0^t \psi(t-t')\theta(t,t')q^+(I,t')dt' - \gamma(t)I(t) + \theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right). \tag{2.11}$$

Further, noting that,

$$\theta(t,0) = \theta(t,t')\theta(t',0) \;\; \forall\, 0 < t' < t, \tag{2.12}$$

we can write Eq. (2.4) as,

$$\frac{I(t)}{\theta(t,0)} = \frac{I_0(t)}{\theta(t,0)} + \int_0^t \phi(t-t')\frac{q^+(I,t')}{\theta(t',0)}dt'. \tag{2.13}$$

As the right hand side contains a convolution, taking the Laplace transform, $\mathcal{L}$, of the equation with respect to time and rearranging gives,

$$\mathcal{L}\left\{\frac{q^+(I,t)}{\theta(t,0)}\right\} = \mathcal{L}\left\{\frac{I(t)}{\theta(t,0)}\right\}\frac{1}{\mathcal{L}\{\phi(t)\}} - \mathcal{L}\left\{\frac{I_0(t)}{\theta(t,0)}\right\}\frac{1}{\mathcal{L}\{\phi(t)\}}. \tag{2.14}$$

This result can then be used to write,

$$\begin{aligned}\int_0^t \psi(t-t')\frac{q^+(I,t')}{\theta(t',0)}dt' &= \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\{\phi(t)\}}\mathcal{L}\left\{\frac{I(t)}{\theta(t,0)}\right\}\right\} - \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\{\phi(t)\}}\mathcal{L}\left\{\frac{I_0(t)}{\theta(t,0)}\right\}\right\}, \\ &= \int_0^t K(t-t')\left(\frac{I(t')}{\theta(t',0)} - \frac{I_0(t')}{\theta(t',0)}\right)dt'.\end{aligned} \tag{2.15}$$

where we have defined the memory kernel,

$$K(t) = \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\{\phi(t)\}}\right\}. \tag{2.16}$$

Equation (2.12) allows us to write Eq. (2.11) as,

$$\frac{dI(t)}{dt} = \omega(t)S(t)I(t) - \theta(t,0)\int_0^t \psi(t-t')\frac{q^+(I,t')}{\theta(t',0)}\,dt' - \gamma(t)I(t) + \theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right), \tag{2.17}$$

which, using Eq. (2.15), becomes,

$$\frac{dI(t)}{dt} = \omega(t)S(t)I(t) - \gamma(t)I(t) - \theta(t,0)\left(\int_0^t K(t-t')\left(\frac{I(t')}{\theta(t',0)} - \frac{I_0(t')}{\theta(t',0)}\right)dt' - \frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right)\right). \tag{2.18}$$

This equation is the generalised master equation that describes the time evolution of the number of infected individuals in an SIR model with arbitrary waiting time in the infectious compartment.

Simple flux balance considerations give the master equations for the other two states. The equations for the susceptible and recovered populations are,

$$\frac{dS(t)}{dt} = \lambda(t) - \omega(t)S(t)I(t) - \gamma(t)S(t), \tag{2.19}$$

$$\frac{dR(t)}{dt} = \theta(t,0)\left(\int_0^t K(t-t')\left(\frac{I(t')}{\theta(t',0)} - \frac{I_0(t)}{\theta(t',0)}\right)dt' - \frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right)\right) - \gamma(t)R(t). \tag{2.20}$$

Equations (2.18), (2.19), and (2.20) are the governing, or generalised master, equations for an SIR model with a general recovery probability.

2.2.1 Relation to the Classic SIR Model

The master equations for the SIR model with a general recovery probability reduce to the classic SIR model equations, with births and deaths, if the probability of not clearing an infection is exponentially distributed, i.e. $\phi(t) = \exp(-\mu t)$. In this case the probability of an individual clearing an infection is not dependent on the amount of time that the person has already been infected. Subsituting the exponential distribution for $\phi(t)$ into the kernel, Eq. (2.16), we obtain,

$$K(t-t') = \mu\delta(t-t'), \tag{2.21}$$

where $\delta(t)$ is the Dirac delta function. Also noting that as $\phi(t) = \exp(-\mu t)$ we can write,

$$\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right) = -\mu\frac{I_0(t)}{\theta(t,0)}. \tag{2.22}$$

We can now substitute the expression for the kernel, Eq. (2.21), into the generalised master equations, Eqs. (2.18), (2.19), and (2.20), to yield the classic SIR equations,

$$\frac{dS(t)}{dt} = \lambda(t) - \omega(t)S(t)I(t) - \gamma(t)S(t), \tag{2.23}$$

$$\frac{dI(t)}{dt} = \omega(t)S(t)I(t) - \mu I(t) - \gamma(t)I(t), \tag{2.24}$$

$$\frac{dR(t)}{dt} = \mu I(t) - \gamma(t)R(t). \tag{2.25}$$

2.2.2 Relation to the Kermack and McKendrick Age-Structured Model

The master equations for the SIR model with a general recovery probability are formally equivalent to a reduction of the general SIR model presented by Kermack and McKendrick [74]. The derivation of the Kermack and McKendrick model from our stochastic process is presented in Appendix A. Here we show how the master equations, Eqs. (2.18), (2.19), (2.20), can be obtained from a reduction of the Kermack and McKendrick SIR model equations given by,

$$\begin{aligned}
\frac{dS}{dt} &= \lambda - \int_0^\infty \omega i(a,t)da S(t) - \gamma S(t), && (2.26)\\
\frac{\partial i}{\partial t} &+ \frac{\partial i}{\partial a} = -\beta(a) i(a,t) - \gamma i(a,t), && (2.27)\\
\frac{dR}{dt} &= \int_0^\infty \beta(a) i(a,t) da - \gamma R(t), && (2.28)\\
I(t) &= \int_0^\infty i(a,t) da. && (2.29)
\end{aligned}$$

In this model $i(a,t)$ is the number of individuals who are infected at time t and who have been infected since time $t-a$. The equivalence can be seen by making the identification,

$$i(a,t) = \Phi(t, t-a) q^+(I, t-a). \tag{2.30}$$

Then Eq. (2.29) is equivalent to Eq. (2.4), provided that the separability assumption, Eq. (2.6), holds. If we assume that $i(a,t) \to 0$ as $a \to \infty$. Integrating Eq. (2.29) with respect to a then gives

$$\frac{dI}{dt} - i(0,t) = -\int_0^\infty \beta(a)\phi(a)\theta(t, t-a) q^+(I, t-a) da - \gamma I. \tag{2.31}$$

Identifying $\beta(a)\phi(a) = \psi(a)$ and $i(0,t) = q^+(I,t)$, we can then split the integral to,

$$\frac{dI}{dt} = i(0,t) - \int_0^t \psi(a)\theta(t, t-a) q^+(I, t-a) da - \int_t^\infty \psi(a)\theta(t, t-a) q^+(I, t-a) da - \gamma I. \tag{2.32}$$

This allows for the use of the same Laplace transform method as in Eqs. (2.14)-(2.18), hence with a change of variable of integration $t' = t - a$ becoming,

$$\frac{dI}{dt} = \omega SI - \theta(t,0)\int_0^t K(t-t')\left(\frac{I(t')}{\theta(t',0)} - \frac{I_0(t')}{\theta(t',0)}\right)dt' + \theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right) - \gamma I. \tag{2.33}$$

Using the result that,

$$\theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right) = -\int_{-\infty}^{0}\psi(t-t')\theta(t,t')q^+(I,t')dt'. \tag{2.34}$$

Hence we have recovered the generalised master equation given in Eq. (2.18) with time independent rates.

2.2.3 Integral Equation Formulation

The master equations for the fractional recovery SIR model can be formulated as a coupled set of integral equations. This enables comparisons with other related models and it enables the application of integral equation methods for analysis of equilibrium states. To formulate the system as integral equations we begin by noting that Eqs. (2.1), (2.3) can be substituted into Eq. (2.4) to yield,

$$q^+(I,t) = \omega(t)S(t)I(t), \tag{2.35}$$

and then Eq. (2.4) can be re-written to obtain the integral equation for the time evolution of the infected state,

$$I(t) = I_0(t) + \int_0^t \Phi(t,t')\omega(t')S(t')I(t')\,dt'. \tag{2.36}$$

The integral equation for the time evolution of the susceptible state can be obtained by direct integration of Eq. (2.19), to yield,

$$S(t) = S(0) + \int_0^t \lambda(t')\,dt' - \int_0^t \omega(t')S(t')I(t')\,dt' - \int_0^t \gamma(t')S(t')\,dt'. \tag{2.37}$$

Note that the total population,

$$N(t) = S(t) + I(t) + R(t), \tag{2.38}$$

and the master equations with a fractional-order recovery were obtained with,

$$\frac{dN}{dt} = \lambda(t) - \gamma(t)N(t). \tag{2.39}$$

We can combine Eqs. (2.38) and (2.39) to obtain the differential equation for the time evolution of the recovery state in the form,

$$\frac{dR}{dt} = -\frac{dI}{dt} - \frac{dS}{dt} + \lambda(t) - \gamma(t)S(t) - \gamma(t)I(t) - \gamma(t)R(t), \tag{2.40}$$

and then integrate to find ,

$$\begin{aligned} R(t) &= R(0) - I(t) + I(0) - S(t) + S(0) + \int_0^t \lambda(t')\,dt' \\ &\quad - \int_0^t \gamma(t')S(t')\,dt' - \int_0^t \gamma(t')I(t')\,dt' - \int_0^t \gamma(t')R(t')\,dt'. \end{aligned} \tag{2.41}$$

After substituting for $I(t)$ and $S(t)$ using Eqs. (2.36) and (2.37) we have the integral equation for the time evolution of the recovered state,

$$\begin{aligned} R(t) &= R(0) + I_0(0) - I_0(t) - \int_0^t \Phi(t,t')\omega(t')S(t')I(t')\,dt' + \int_0^t \omega(t')S(t')I(t')\,dt' \\ &\quad - \int_0^t \gamma(t')I(t')\,dt' - \int_0^t \gamma(t')R(t')\,dt'. \end{aligned} \tag{2.42}$$

Equations (2.37), (2.36) and (2.42), provide a general set of coupled integral equations for fractional recovery SIR models. The integral equation for the susceptible state, Eq. (2.47), can be shown to be equivalent to the integral equation obtained from $S(t) = N(t) - I(t) - R(t)$ in the special case where $\lambda(t) = \gamma(t)N(t)$, and thus $N(t) = N(0)$ is constant.

2.2.4 Reduction to the Hethcote and Tudor Endemic Disease Model

If $\gamma(t), \omega(t)$ and $\lambda(t)$ are constant in time then the integral equations, (2.37), (2.36), (2.42) reduce to the integral equation model for endemic infection diseases that was introduced by Hethcote and Tudor [65].

We first note that, with γ constant,

$$\Phi(t, t') = \phi(t - t')e^{-\gamma(t-t')}, \tag{2.43}$$

and,

$$\frac{dY(t)}{dt} + \gamma Y(t) = e^{-\gamma t}\frac{d}{dt}\left(e^{\gamma t}Y(t)\right), \tag{2.44}$$

Substituting Eq. (2.43) into Eq. (2.36), with ω also constant, we have,

$$I(t) = I_0(t) + \int_0^t \phi(t - t')e^{-\gamma(t-t')}\omega S(t')I(t')\,dt'. \tag{2.45}$$

Using Eq. (2.44) we can re-write Eq. (2.19), with ω, γ and λ constant as,

$$\frac{d}{dt}\left(e^{\gamma t}S(t)\right) = e^{\gamma t}\lambda - e^{\gamma t}\omega S(t)I(t), \tag{2.46}$$

and then integrate with respect to time to obtain,

$$S(t) = e^{-\gamma t}S(0) + \int_0^t e^{-\gamma(t-t')}\lambda\,dt' - \int_0^t e^{-\gamma(t-t')}\omega S(t')I(t')\,dt'. \tag{2.47}$$

Using Eq. (2.44) we can re-write Eq. (2.40), with ω, γ and λ constant as,

$$\frac{d}{dt}\left(e^{\gamma t}R(t)\right) = \lambda e^{\gamma t} - \frac{d}{dt}\left(e^{\gamma t}S(t)\right) - \frac{d}{dt}\left(e^{\gamma t}I(t)\right), \tag{2.48}$$

and then integrate with respect to time to obtain,

$$R(t) = R(0)e^{-\gamma t} - I(t) + I(0)e^{-\gamma t} - S(t) + S(0)e^{-\gamma t} + \int_0^t \lambda e^{-\gamma(t-t')}\,dt'. \tag{2.49}$$

We now substitute for $I(t)$ and $S(t)$ using Eqs. (2.45), (2.47) to obtain,

$$R(t) = R(0)e^{-\gamma t} + I_0(0)e^{-\gamma t} - I_0(t) + \int_0^t \omega S(t')I(t')e^{-\gamma(t-t')}\left(1-\phi(t-t')\right)\,dt'. \quad (2.50)$$

Equations (2.45) and (2.50) recover the integral equations for the infected state and the recovery state in the endemic infection diseases model introduced in [65]. The integral equation for the susceptible state in this case can be shown to be equivalent to the integral equation obtained from $S(t) = N - I(t) - R(t)$ with $N(t) = N(0) = \lambda/\gamma$.

2.3 Fractional Recovery SIR Model

When a person is persistently infected for a long period period of time, with little chance of spontaneous recovery, they are said to be chronically infected. This type of behaviour is not captured by the assumptions of the standard SIR model, i.e., exponentially distributed waiting times. We can incorporate chronic infections by having, at least asymptotically, the rate of clearing the disease decrease with the amount of time that an individual has been infected. In this case the 'hazard rate', $h(t)$, defined as the rate of recovering at time t conditional on surviving until time t, will be a monotonically decreasing function. In general we can write the hazard rate as,

$$h(t) = \frac{\psi(t)}{\phi(t)}. \quad (2.51)$$

All power-law tailed distributions have an asymptoticly decreasing hazard rate. In the tail of the distribution $\psi(t) \sim \alpha t^{-\alpha-1}$ and $\phi(t) \sim t^{-\alpha}$. Hence the hazard rate will asymptote to $\frac{\alpha}{t}$, which is a monotonically decreasing function. As such a power-law tailed waiting time distribution may be an appropriate distribution in modelling chronic infections, although it is not the only choice for distributions with a decreasing hazard rate. If we consider a power-law exponent $\alpha < 1$ then the first moment of the distribution will not exist, and the expected waiting time will diverge. Thus

using a power-law tailed waiting time distribution in our SIR model can lead to some individuals becoming "trapped" in the infectious compartment until they die.

We will take the power-law tailed Mittag-Leffler distribution as our waiting time distribution. Using this distribution our general SIR model will reduce to a set of differential equations with a fractional-order time derivative on the recovery transition.

The Mittag-Leffler probability density is defined by [67],

$$\psi(t) = \frac{t^{\alpha-1}}{\tau^{\alpha}} E_{\alpha,\alpha}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right), \tag{2.52}$$

with $0 < \alpha \leq 1$. Here $E_{\alpha,\beta}(z)$ is the two parameter Mittag-Leffler function, defined by,

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha+\beta)}. \tag{2.53}$$

The Mittag-Leffler distribution limits to an exponential distribution in the case $\alpha = 1$. For $0 < \alpha < 1$ the density has a power-law tail at long times [29],

$$\psi(t) \sim t^{-1-\alpha}. \tag{2.54}$$

The corresponding survival function is given by,

$$\phi(t) = E_{\alpha,1}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right). \tag{2.55}$$

The Laplace transform from t to s of the memory kernel, Eq. (2.16), for a Mittag-Leffler distribution is given by,

$$\mathcal{L}_t[K(t)|s] = s^{1-\alpha}\tau^{-\alpha}. \tag{2.56}$$

Here we use the notation $\mathcal{L}_t[Y(t)|s]$ to denote the Laplace transform of $Y(t)$ from t to s and we use the notation $\mathcal{L}_s^{-1}[Y(s)|t]$ to denote the inverse Laplace transform of

$Y(s)$ from s to t. Without loss of generality we define,

$$\mu = \tau^{-\alpha}. \tag{2.57}$$

We also recall that the Riemann-Liouville fractional derivative, defined by Eq. (1.8) for $0 < \alpha < 1$ is,

$${}_0\mathcal{D}_t^{1-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \frac{d}{dt} \int_0^t \frac{f(t')}{(t-t')^{1-\alpha}}\, dt'. \tag{2.58}$$

The Laplace transform, defined in Eq. (1.9), can be expressed as,

$$\mathcal{L}_t[\,{}_0\mathcal{D}_t^{1-\alpha} f(t)|s] = s^{1-\alpha}\mathcal{L}_t[f(t)|s], \tag{2.59}$$

for sufficiently smooth $f(t)$. The fractional derivative can also be written as the following convolution,

$${}_0\mathcal{D}_t^{1-\alpha} f(t) = \int_0^t \mathcal{L}_s^{-1}\left[s^{1-\alpha}\middle|t'\right] f(t-t')dt'. \tag{2.60}$$

It follows from Eq. (2.56) and Eq. (2.60) that if the kernel in Eqs. (2.18), (2.19), (2.20) is obtained from the Mittag-Leffler waiting time density then we obtain the generalised master equations with fractional recovery,

$$\frac{dS(t)}{dt} = \lambda(t) - \omega(t)S(t)I(t) - \gamma(t)S(t), \tag{2.61}$$

$$\frac{dI(t)}{dt} = \omega(t)S(t)I(t) - \gamma(t)I(t) - \theta(t,0)\left(\mu\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)} - \frac{I_0(t)}{\theta(t,0)}\right) - \frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right)\right), \tag{2.62}$$

$$\frac{dR(t)}{dt} = \theta(t,0)\left(\mu\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)} - \frac{I_0(t)}{\theta(t,0)}\right) - \frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right)\right) - \gamma(t)R(t). \tag{2.63}$$

In the following we will refer to the above set of equations as the fractional recovery SIR model. Letting $\alpha = 1$ recovers the standard SIR model.

2.3.1 Equilibrium States

The fractional recovery SIR model is a non-autonomous dynamical system which can be simplified, by taking the birth, infectivity and death rate to be constant parameters, $\lambda(t) = \lambda$, $\omega(t) = \omega$ and $\gamma(t) = \gamma$ respectively, giving,

$$\frac{dS(t)}{dt} = \lambda - \omega S(t)I(t) - \gamma S(t), \tag{2.64}$$

$$\frac{dI(t)}{dt} = \omega S(t)I(t) - \gamma I(t) - e^{-\gamma t}\left(\mu\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t}\left(I(t) - I_0(t)\right)\right) - \frac{d}{dt}\left(e^{\gamma t} I_0(t)\right)\right), \tag{2.65}$$

$$\frac{dR(t)}{dt} = e^{-\gamma t}\left(\mu\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t}\left(I(t) - I_0(t)\right)\right) - \frac{d}{dt}\left(e^{\gamma t} I_0(t)\right)\right) - \gamma R(t). \tag{2.66}$$

We take the equilibrium state to be (S^*, I^*, R^*), such that,

$$\lim_{t\to\infty} S(t) = S^*, \qquad \lim_{t\to\infty} I(t) = I^*, \qquad \lim_{t\to\infty} R(t) = R^*. \tag{2.67}$$

Taking the limit as $t \to \infty$ of Eqs. (2.64), (2.65), and (2.66), and noting that,

$$\lim_{t\to\infty} I_0(t) = 0, \ \lim_{t\to\infty} \frac{d}{dt}\left(e^{\gamma t} I_0(t)\right) = 0. \tag{2.68}$$

we have

$$0 = \lambda - \omega S^* I^* - \gamma S^*, \tag{2.69}$$

$$0 = \omega S^* I^* - \lim_{t\to\infty} e^{-\gamma t}\mu\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t}\left(I(t) - I_0(t)\right)\right), \tag{2.70}$$

$$0 = \lim_{t\to\infty} e^{-\gamma t}\mu\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t}\left(I(t) - I_0(t)\right)\right) - \gamma R^*. \tag{2.71}$$

In order to calculate the unevaluated limits in Eqs. (2.70), and (2.71) we consider a Laplace transform of the terms,

$$\mathcal{L}\{e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t} J(t)\right)\} = (s+\gamma)^{1-\alpha}\left(\hat{J}(s)\right). \tag{2.72}$$

In which we have defined,

$$J(t) = I(t) - I_0(t). \tag{2.73}$$

We can express Eq. (2.72) using a Taylor series expansion,

$$\hat{J}(s)(s+\gamma)^{1-\alpha} = \hat{J}(s)\left(\gamma^{1-\alpha} + (1-\alpha)\gamma^{-\alpha}s + O(s^2)\right). \tag{2.74}$$

As the Laplace transform is a linear operator we can take the inverse termwise, producing,

$$e^{-\gamma t}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t}(I(t) - I_0(t))\right) = \mathcal{L}^{-1}\{\hat{J}(s)\left(\gamma^{1-\alpha} + (1-\alpha)\gamma^{-\alpha}s + O(s^2)\right)\}, \tag{2.75}$$

$$= \gamma^{1-\alpha}J(t) + (1-\alpha)\gamma^{-\alpha}\frac{dJ(t)}{dt} + \mathcal{L}^{-1}\left(O(s^2)\right). \tag{2.76}$$

The limit of $J(t)$ is,

$$\lim_{t\to\infty} J(t) = I^*. \tag{2.77}$$

It is then clear that, in the long time limit, the inverse Laplace transform of the higher order terms of the Taylor expansion will become zero, i.e.

$$\lim_{t\to 0}\frac{dJ(t)}{dt} = 0, \tag{2.78}$$

$$\lim_{t\to 0}\mathcal{L}^{-1}\left(O(s^2)\right) = 0. \tag{2.79}$$

Thus we can compute the desired limit,

$$\lim_{t\to\infty} e^{-\gamma t}\,{}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t}\left(I(t) - I_0(t)\right)\right) = \gamma^{1-\alpha}I^*. \tag{2.80}$$

Substituting Eq. (2.80) into Eqs. (2.64), (2.65), and (2.66) yields,

$$0 = \lambda - \omega S^* I^* - \gamma S^*, \tag{2.81}$$

$$0 = \omega S^* I^* - \mu\gamma^{1-\alpha} I^* - \gamma I^*, \tag{2.82}$$

$$0 = \mu\gamma^{1-\alpha} I^* - \gamma R^*. \tag{2.83}$$

Solving Eqs. (2.81), (2.82), and (2.83) reveals two equilibrium states, the disease free state,

$$S^* = \frac{\lambda}{\gamma}, \quad I^* = 0, \quad R^* = 0, \tag{2.84}$$

and the endemic state,

$$S^* = \frac{\mu\gamma^{1-\alpha} + \gamma}{\omega}, \quad I^* = \frac{\lambda}{\mu\gamma^{1-\alpha} + \gamma} - \frac{\gamma}{\omega}, \quad R^* = \frac{\mu\lambda}{\mu\gamma + \gamma^{1+\alpha}} - \frac{\mu\gamma^{1-\alpha}}{\omega}. \tag{2.85}$$

As the population in each compartment can not be negative the endemic equilibrium can only exist if,

$$\lambda\omega > \mu\gamma^{2-\alpha} + \gamma^2. \tag{2.86}$$

When $\alpha = 1$, the equilibrium states are equivalent to the fixed points of the classic SIR model with constant parameters. For $0 < \alpha < 1$ the equilibrium states are not fixed points. This invalidates the use of a standard linear stability analysis around the equilibrium states. However some progress can be made by considering the integral equation formulation of the fractional recovery SIR model, Eqs. (2.45), (2.47), and (2.50). After a translation of the equilibrium states to the origin, the asymptotic behaviour of the resulting system of nonlinear Volterra integral equations is equivalently given by the asymptotic behaviour of its linearisation as a system of linear Volterra integral equations [108]. This result was used by Hethcote and Tudor [65] to infer local stability properties of the equilibrium states of the integral equations Eqs. (2.45), (2.47), and (2.50). If the results of Hethcote and Tudor [65] are applied to the special case of the fractional recovery SIR model, where $\phi(t)$ is

defined in Eq. (2.55), then the disease free state, Eq. (2.84), is locally stable if $\lambda\omega \leq \mu\gamma^{2-\alpha} + \gamma^2$ and the endemic equilibrium state, Eq. (2.85), is locally stable when it exists.

2.4 Summary

We have derived a fractional recovery SIR model that differs from the classic SIR model by considering the case where the recovery from a disease does not follow an exponential distribution, but follows a distribution with a power-law tail. The fractional-order model is biologically motivated by the observation that in some disease processes, the longer a person is infectious the more likely they will remain infectious. The fractional-order model permits both a disease free equilibrium state and an endemic equilibrium state. We have related the fractional-order model to the generalised SIR models introduced by Kermack and McKendrick. The fractional-order model that we have derived is different to *ad hoc* fractional epidemic models and avoids dimensionality and flux-balance problems. While we have focused on the derivation of a fractional-order recovery SIR throughout this chapter, we consider the conditions necessary to result in a fractional-order infectivity SIR model in Chapter 4. Additionally, the derivation of a combined fractional infectivity and fractional recovery SIR model is discussed Chapter 5. It is natural to extend the derivation of fractional-order recovery SIR model, outside of epidemic applications, to a general fractional compartment model, which is considered in Chapter 3.

Chapter 3

General Fractional Compartment Model

3.1 Introduction

This Chapter is based on the publication [14]. In this Chapter we derive a general framework for formulating fractional-order compartment models, by considering the governing equations from an underlying stochastic processes. The stochastic process models particles entering a compartment, waiting for a random time, and then leaving the compartment. The governing equations we derive describe the time evolution of an ensemble of particles that are undergoing this process. If the particles that leave one compartment always enter another compartment the stochastic process is equivalent to a generalised CTRW [111] with waiting times moderating transitions between compartments. As such, this formalism for the compartment model dynamics further extends the theory of CTRWs with reactions [62, 53, 158, 7, 114] and it generalizes recent work on fractional-order SIR models [21, 20], presented in Chapters 2 and 4. Fractional-order compartment models are obtained when the waiting time in a compartment is governed by a non-Markovian process, whereby the probability of leaving the compartment is dependent on the length of time spent in the compartment. The fractional models can be formulated as age structured integro-differential models, however the formulation using fractional derivatives enables ready comparison with the growing literature on fractional-order compartment models. Moreover the age structured integro-differential models can be derived from the underlying stochastic processes considered here.

The remainder of this Chapter is organized as follows: In Section 3.2, starting with a stochastic process, we derive the governing equation for an ensemble of particles in a single compartment. This is reduced to a fractional-order differential equation by considering a power-law distribution for the time that a particle remains in the compartment. fractional-order multi-compartment models can be constructed by linking multiple fractional-order single compartment models. Details on this are provided in Sections 3.3, and in Section 3.4, examples of fractional-order multi-compartment models are developed.

3.2 Single Compartment Model

In order to develop a general compartment model we first consider the dynamics of a single compartment. We derive a generalised master equation that describes the population of the compartment through time, and show the assumptions that lead to fractional dynamics. We will then combine multiple single compartments together to form the general model.

In a single compartment we consider an ensemble of particles. We assume that each member of this ensemble is undergoing a stochastic process in which; they are created, they last for a random amount of time, and then they are removed from the compartment. In general, new particles can be created in this ensemble by a number of distinct creation processes, and similarly particles can be removed from the ensemble by a number of distinct removal processes.

We assume that the creation of the particles in the ensemble is governed by N_C distinct creation processes. In the mean field, the arrival flux of particles due to the i^{th} creation process is labeled $\beta_i(t)$. The expected number of particles created in the compartment by the creation process between times t and $t + \delta t$, is $\beta_i(t)\delta t + o(\delta t)$. The total arrival flux, $q(t)$, is the sum of the fluxes due to the creation processes,

$$q(t) = \sum_{i=1}^{N_{\text{C}}} \beta_i(t)\,. \tag{3.1}$$

A particle remains in a compartment until removed by one of the removal processes. We allow for an arbitrary number N_R of *Markovian* removal processes where the probability of a particle being removed from the ensemble at time t only depends on the state of the system at time t. For each individual Markovian removal process, the probability of surviving, from time t_0 to t, is $\Lambda_i(t, t_0)$. The probability of surviving all Markovian removal processes from time t_0 to t is then given by $\Theta(t, t_0) = \prod_{i=1}^{N_R} \Lambda_i(t, t_0)$. As a particle can not be created and removed in the same instance we have $\Theta(t_0, t_0) = 1$.

In general, the probability that a particle will be removed by the i^{th} Markovian removal process in the time interval t to $t + \delta t$ will be $\lambda_i(t)\delta t + o(\delta t)$. This allows us to write the survival function as,

$$\Theta(t, t_0) = \exp\left(-\int_{t_0}^{t} \omega(s) ds\right). \tag{3.2}$$

where,

$$\omega(t) = \sum_{i=1}^{N_R} \lambda_i(t). \tag{3.3}$$

From this we can see that the Markovian survival function must obey the semi-group property,

$$\Theta(t, t_0) = \Theta(t, u)\Theta(u, t_0)\,, \tag{3.4}$$

for any $t_0 \leq u \leq t$. And furthermore,

$$\frac{\mathrm{d}\Theta(t, t_0)}{\mathrm{d}t} = -\omega(t)\Theta(t, t_0)\,. \tag{3.5}$$

We also include a *non-Markovian* removal process, where the probability that a particle is removed from the ensemble is dependent on the length of time since the particle entered the compartment, i.e. if the particle entered the compartment at time t_0 the process at time t will be dependent on the variable $t - t_0$. The survival probability for the non-Markovian removal process is given by $\Phi(t)$, and we require

that $\Phi(0) = 1$. It can be expressed in terms of a waiting time density, $\phi(t)$,

$$\Phi(t) = 1 - \int_0^t \phi(u)\,\mathrm{d}u\,. \tag{3.6}$$

The waiting time density $\phi(t)$ gives the likelihood of waiting in a compartment for a length of time t having arrived at time 0. From Eq. (3.6) the derivative of the survival function is,

$$\frac{d\Phi(t)}{dt} = -\phi(t). \tag{3.7}$$

For a particle to be in the compartment at time t it must have entered the compartment at some earlier time t_0, and survived until time t. We assume that the various removal processes are independent and hence can say that the probability of surviving all of the removal processes, given an arrival time of t_0, is given by $\Phi(t - t_0)\Theta(t, t_0)$. Thus the number of particles in the compartment at time t, $\rho(t)$, can be written,

$$\rho(t) = \int_0^t \Phi(t - t_0)\Theta(t, t_0)\, q(t_0)\,\mathrm{d}t_0\,. \tag{3.8}$$

We have assumed that there are no particles in the compartment before time zero, i.e. $\rho(t) = 0$ for $t < 0$.

To obtain a differential equation that governs the dynamics of the number of particles in the compartment we take the derivative of ρ. This can be done by using Leibniz rule for differentiating under the integral sign provided that the integrand is continuous [7]. Here, we wish to consider the case where there can be an injection of flux into the compartment at time $t = 0$, with the flux a continuous function for $t > 0$. Thus we write,

$$q(t) = i_0\delta(t - 0^+) + q^+(t), \tag{3.9}$$

where i_0 is the initial injection and $q^+(t)$ is right continuous at $t = 0$ and continuous for all $t > 0$. Substituting Eq. (3.9) into Eq. (3.8) we can write,

$$\rho(t) = i_0\Phi(t)\Theta(t, 0) + \int_0^t \Phi(t - t_0)\Theta(t, t_0)\, q^+(t_0)\,\mathrm{d}t_0\,, \tag{3.10}$$

this ensures that the integrand is continuous for continuous survival functions. Taking the derivative of Eq. (3.10), applying the Leibniz rule and using Eqs. (3.5) and (3.7), we find that,

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = q^{+}(t) - \omega(t)\rho(t) - F_{\phi}(t), \tag{3.11}$$

where we have defined,

$$F_{\phi}(t) = \int_{0}^{t} \phi(t - t_0)\Theta(t, t_0)q(t_0)\,\mathrm{d}t_0\,, \tag{3.12}$$

which denotes the outgoing flux due to the non-Markovian process. The outgoing flux $F_{\phi}(t)$ can be expressed in terms of ρ by using Laplace transform techniques. We divide Eqs. (3.8) and (3.12) by $\Theta(t, 0)$, and using the semi-group property, Eq. (3.4), we find,

$$\frac{\rho(t)}{\Theta(t,0)} = \int_{0}^{t} \Phi(t - t_0)\,\frac{q(t_0)}{\Theta(t_0,0)}\,\mathrm{d}t_0, \tag{3.13}$$

$$\frac{F_{\phi}(t)}{\Theta(t,0)} = \int_{0}^{t} \phi(t - t_0)\,\frac{q(t_0)}{\Theta(t_0,0)}\,\mathrm{d}t_0\,. \tag{3.14}$$

As both these equations are convolutions, taking the Laplace transform gives,

$$\mathcal{L}_t\left\{\frac{\rho(t)}{\Theta(t,0)}\right\} = \mathcal{L}_t\{\Phi(t)\}\,\mathcal{L}_t\left\{\frac{q(t)}{\Theta(t,0)}\right\}, \tag{3.15}$$

$$\mathcal{L}_t\left\{\frac{F_{\phi}(t)}{\Theta(t,0)}\right\} = \mathcal{L}_t\{\phi(t)\}\,\mathcal{L}_t\left\{\frac{q(t)}{\Theta(t,0)}\right\}. \tag{3.16}$$

Re-arranging Eq. (3.15) and substituting into Eq. (3.16), we simplify this to

$$\mathcal{L}_t\left\{\frac{F_{\phi}(t)}{\Theta(t,0)}\right\} = \mathcal{L}_t\{K(t)\}\,\mathcal{L}_t\left\{\frac{\rho(t)}{\Theta(t,0)}\right\}, \tag{3.17}$$

where we have defined the *memory kernel* $K(t)$ as,

$$\mathcal{L}_t\{K(t)\} = \frac{\mathcal{L}_t\{\phi(t)\}}{\mathcal{L}_t\{\Phi(t)\}}\,. \tag{3.18}$$

Taking the inverse Laplace transform of Eq. (3.17) allows us to express $F_\phi(t)$ as,

$$F_\phi(t) \;=\; \int_0^t K(t-t_0)\,\Theta(t,t_0)\,\rho(t_0)\,\mathrm{d}t_0\,. \tag{3.19}$$

Using Eq. (3.19) in Eq. (3.11) we write,

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = q^+(t) - \omega(t)\rho(t) - \int_0^t K(t-t_0)\Theta(t,t_0)\rho(t_0)\,\mathrm{d}t_0. \tag{3.20}$$

This is the governing equation for an ensemble of particles in a single compartment, where the particles are created and removed by underlying stochastic processes. This equation is true for an arbitrary waiting time distribution for the non-Markovian removal process. The formulation of Eq. (3.11) relies on the history of $q(t)$ while Eq. (3.20) relies on the history of $\rho(t)$. We shall show that, with the appropriate choice of a waiting time distribution, the convolution over the memory kernel may be expressed as a fractional derivative.

3.2.1 Relationship to Age-Structured Models

Age-structured compartment models [73, 102, 38] allow for the dynamics of the system to depend on 'system' time, as well as the length of time particles have been in a particular compartment. The governing evolution equation for age structured dynamics can be shown to be equivalent to the governing evolution equation for an ensemble of particles in a single compartment, where the particles are created and removed by underlying stochastic processes. Moreover the governing evolution equation for age structured dynamics can be derived from the underlying stochastic process. In the derivations below we consider the simplification in which the arrival density $q(t)$ is continuous for $t \geq 0$.

3.2.1.1 Derivation of Age-Structured Dynamics from an Underlying Stochastic Process

Considering the underlying stochastic process for single compartment dynamics introduced in Section II we define $\widehat{\rho}(t,a)$ as the number density of particles in the compartment at time t with age a. Similar to Eq. (3.8) this is given by

$$\widehat{\rho}(t,a) = \int_0^t \Phi(t-t_0)\Theta(t,t_0)q(t_0)\delta(t-t_0,a)\ dt_0, \tag{3.21}$$

where the delta function has been introduced to select those particles that arrived in the compartment at time t_0 and have age a at time t. The integral over all times t_0 leads to

$$\widehat{\rho}(t,a) = \Phi(a)\Theta(t,t-a)q(t-a). \tag{3.22}$$

The evolution equation for the age-structured number density can now be found by differentiating Eq. (3.21) with respect to time. This results in

$$\begin{aligned}\frac{\partial\widehat{\rho}(t,a)}{\partial t} + \frac{\partial\widehat{\rho}(t,a)}{\partial a} &= \frac{d\Phi(a)}{da}\Theta(t,t-a)q(t-a) \\ &\quad +\Phi(a)q(t-a)\left(\frac{\partial}{\partial t}\Theta(t,t-a) + \frac{\partial}{\partial a}\Theta(t,t-a)\right),\end{aligned} \tag{3.23}$$

where we have used the results that

$$\frac{dt}{dt} = \frac{da}{dt} = 1,$$

and

$$\frac{\partial}{\partial t}q(t-a) = -\frac{\partial}{\partial a}q(t-a).$$

In general we can write the survival function as

$$\Phi(a) = \exp\left(-\int_0^a \gamma(s)\,ds\right), \tag{3.24}$$

where

$$\gamma(a) = \frac{\psi(t)}{\Phi(t)} \tag{3.25}$$

is the associated hazard rate dependent on age [21]. Furthermore, recalling

$$\Theta(t, t-a) = \exp\left(-\int_{t-a}^{t} \omega(s)ds\right), \tag{3.26}$$

it is a simple exercise to show that

$$\frac{\partial}{\partial t}\Theta(t, t-a) + \frac{\partial}{\partial a}\Theta(t, t-a) = -\omega(t)\Theta(t, t-a), \tag{3.27}$$

and using Eq. (3.24),

$$\frac{d\Phi}{da} = -\gamma(a)\Phi(a). \tag{3.28}$$

We can now substitute Eqs. (3.28) and (3.27) into Eq. (3.23) and simplify, using Eq. (3.22), to obtain

$$\frac{\partial\widehat{\rho}(t,a)}{\partial t} + \frac{\partial\widehat{\rho}(t,a)}{\partial a} = -\gamma(a)\widehat{\rho}(t,a) - \omega(t)\widehat{\rho}(t,a), \tag{3.29}$$

which is the governing evolution equation for the number density of particles in an age-structured model. The terms on the right hand side of this equation identify a non-Markovian removal process dependent on the age of the particle, with a corresponding rate $\gamma(a)$ and a Markovian removal process with rate $\omega(t)$. It also follows from Eqs. (3.22), (3.24) and (3.26) that

$$\widehat{\rho}(t, 0) = q(t), \tag{3.30}$$

so that the flux from creation processes, $q(t)$, are incorporated into the model as a boundary condition. The governing equation, Eq. (3.29), encompasses models such as Kermack and McKendrick's structured SIR model [73].

3.2.2 From Age-Structured Dynamics to Stochastic Compartment Dynamics

We can obtain the evolution equation for the stochastic compartment dynamics from the governing evolution equation for the number density of particles in an age-structured model. First we note that

$$\rho(t) = \int_0^t \widehat{\rho}(t,a)\, da. \tag{3.31}$$

As $q(t)$ is continuous $\widehat{\rho}(t,a)$ is also continuous and we can differentiate with respect to time using Leibniz rule, to arrive at

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = \int_0^t \frac{\partial\widehat{\rho}(t,a)}{\partial t}\mathrm{d}a + \widehat{\rho}(t,t). \tag{3.32}$$

Taking the integral of the evolution equation for age-structured dynamics, Eq. (3.29), with respect to a, we obtain,

$$\int_0^t \frac{\partial\widehat{\rho}(t,a)}{\partial t}\mathrm{d}a + \widehat{\rho}(t,t) - \widehat{\rho}(t,0) = -\omega(t)\int_0^t \widehat{\rho}(t,a)\,\mathrm{d}a - \int_0^t \gamma(a)\widehat{\rho}(t,a)\,\mathrm{d}a. \tag{3.33}$$

The results in Eqs. (3.31), (3.32) and (3.33) can be combined to arrive at

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} - \widehat{\rho}(t,0) = -\omega(t)\rho(t) - \int_0^t \gamma(a)\widehat{\rho}(t,a)\,\mathrm{d}a. \tag{3.34}$$

We now replace $\widehat{\rho}(t,a)$ and $\widehat{\rho}(t,0)$ using Eqs. (3.22) and (3.30) respectively. This results in

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = q(t) - \omega(t)\rho(t) - \int_0^t \gamma(a)\Phi(a)\Theta(t,t-a)q(t-a)\,da, \tag{3.35}$$

and after a change of variables $a = t - t_0$,

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = q(t) - \omega(t)\rho(t) - \int_0^t \gamma(t-t_0)\Phi(t-t_0)\Theta(t,t_0)q(t_0)\,\mathrm{d}t_0. \tag{3.36}$$

It follows from Eq. (3.25) that

$$\gamma(t-t_0)\Phi(t-t_0) = \phi(t-t_0), \tag{3.37}$$

so that we can use the same sequence of steps as Eqs. (3.15) - (3.19) to arrive at the governing evolution equation for stochastic compartment dynamics

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = q(t) - \omega(t)\rho(t) - \int_0^t K(t-t_0)\Theta(t,t_0)\rho(t_0)\,\mathrm{d}t_0, \tag{3.38}$$

which is equivalent to Eq. (3.20) in the case on continuous $q(t)$.

3.2.3 Fractional-order Single Compartment Model

The inclusion of a fractional derivative in the governing equations requires a power-law tailed waiting time distribution for the non-Markovian removal process. The use of such a distribution implies that the longer particles have been in a compartment the slower their rate of removal by this process. If there are no other removal processes, this is akin to particles becoming trapped in the compartment as the expected time until removal diverges. To obtain the fractional derivatives at all times, rather then simply asymptotically, we will take the non-Markovain waiting time to be Mittag-Leffler distributed. This distribution has a power-law asymptotic decay [29] as $t \to \infty$, i.e. $\phi(t) \sim t^{-1-\alpha}$. The survival function of a Mittag-Leffler distribution was introduced in Chapter 2, Eq. (2.55). We have written it again here for convenience,

$$\Phi(t) = E_{\alpha,1}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right), \tag{3.39}$$

for an exponent $0 < \alpha \leq 1$, and time scale parameter $\tau > 0$. Taking the Laplace transform of the Mittag-Leffler survival function from t to s gives,

$$\mathcal{L}_t\{\Phi(t)\} = \frac{1}{s(1+(\tau s)^{-\alpha})}. \tag{3.40}$$

The Laplace transform of the corresponding memory kernel K, calculated from Eq. (3.18), is,

$$\mathcal{L}_t\{K(t)\} = \tau^{-\alpha} s^{1-\alpha}, \tag{3.41}$$

where we have used Eq. (3.6) and the fact that $\mathcal{L}_t\{\phi\} = 1 - s\mathcal{L}_t\{\Phi\}$.

Again using Laplace transforms we can rewrite the outgoing flux due to the non-Markovian removal process, $F_\phi(t)$, as,

$$\begin{aligned} F_\phi(t) &= \int_0^t K(t-t_0)\Theta(t,t_0)\,\rho(t_0)\,\mathrm{d}t_0, \\ &= \Theta(t,0)\int_0^t K(t-t_0)\,\frac{\rho(t_0)}{\Theta(t_0,0)}\,\mathrm{d}t_0, \\ &= \Theta(t,0)\mathcal{L}_s^{-1}\left\{\tau^{-\alpha}s^{1-\alpha}\mathcal{L}_t\left\{\frac{\rho(t)}{\Theta(t,0)}\right\}\right\}. \end{aligned} \tag{3.42}$$

This Laplace space representation of the flux can be related to a Riemann-Liouville fractional derivative, allowing us to write the governing equation as a fractional-order differential equation.

The Laplace transform of the Riemann-Liouville fractional derivative, from Eq. (1.9), is in this case,

$$\mathcal{L}_t\{\,{}_0\mathcal{D}_t^{1-\alpha} f(t)\} = s^{1-\alpha}\mathcal{L}_t\{f(t)\} - \,{}_0\mathcal{D}_t^{-\alpha} f(t)|_0. \tag{3.43}$$

We assume that $f(t) = \frac{\rho(t)}{\Theta(t,0)}$ is continuous for $t \geq 0$ in which case we have [89],

$${}_0\mathcal{D}_t^{-\alpha}\left(\frac{\rho(t)}{\Theta(t,0)}\right)\Big|_0 = 0. \tag{3.44}$$

Using Eq. (3.43) we can simplify Eq. (3.42) to,

$$F_\phi(t) = \tau^{-\alpha}\Theta(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{\rho(t)}{\Theta(t,0)}\right). \tag{3.45}$$

Finally, substituting this into Eq. (3.20), we have,

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = q^{+}(t) - \omega(t)\rho(t) - \tau^{-\alpha}\Theta(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{\rho(t)}{\Theta(t,0)}\right). \tag{3.46}$$

This is the fractional-order governing equation for a single compartment model. We will use this to construct general compartment models. It should be noted that the regularity condition given in Eq. (3.44) can be relaxed by considering a Grünwald-Letnikov derivative in place of the Riemann-Liouville derivative, see for example [158].

3.2.4 Equilibrium State Analysis

The inclusion of the fractional derivative leads to some complication with the calculation of equilibrium states. This is due to the fact that the Riemann-Liouville derivate of a constant is non-zero. A further complication is the explicit t dependence in the $\Theta(t,0)$ function. As such, to find the equilibrium behaviour of the model we need to consider the behaviour of solutions as $t \to \infty$. The system approaches an equilibrium solution if the limit,

$$\lim_{t\to\infty} \rho(t) = \rho^{*}, \tag{3.47}$$

exists. It should be noted that this limit may be dependent on the initial condition of the system, and hence multiple equilibrium solutions are possible. The first requirement for the existence of an equilibrium is that the rates associated with the Markovian removal processes and the incoming flux all approach a constant as $t \to \infty$, i.e.

$$\lim_{t\to\infty} \omega(t) = \omega^{*}, \tag{3.48}$$

$$\lim_{t\to\infty} q^{+}(t) = q^{*}. \tag{3.49}$$

For simplicity we will consider the case where $\omega(t) = \omega^*$ for all time so that,

$$\Theta(t,0) = \exp\left(-\omega^* t\right). \tag{3.50}$$

Consider the limit of Eq. (3.46),

$$\lim_{t\to\infty} \frac{\mathrm{d}\rho}{\mathrm{d}t} = \lim_{t\to\infty} \left(q^+(t) - \omega(t)\rho(t) - \tau^{-\alpha}\Theta(t,0)\, {}_0\mathcal{D}_t^{1-\alpha}\left(\frac{\rho(t)}{\Theta(t,0)}\right)\right). \tag{3.51}$$

From Eq. (3.47) the left hand side is zero, and the first two terms on the right hand side simplify trivially leaving,

$$0 = q^* - \omega^*\rho^* - \tau^{-\alpha} \lim_{t\to\infty} \exp\left(-\omega^* t\right)\, {}_0\mathcal{D}_t^{1-\alpha}\left(\exp\left(\omega^* t\right)\rho(t)\right). \tag{3.52}$$

To evaluate the last term on the right hand side of Eq. (3.52), we take the Laplace transform, and apply the well known shift identity, as well as the binomial expansion, to yield

$$\begin{aligned}
\mathcal{L}_t\left\{\exp\left(-\omega^* t\right)\, {}_0\mathcal{D}_t^{1-\alpha}\left(\exp\left(\omega^* t\right)\rho(t)\right)\right\} &= \mathcal{L}_t\left\{\, {}_0\mathcal{D}_t^{1-\alpha}\left(\exp\left(\omega^* t\right)\rho(t)\right); s+\omega^*\right\} \\
&= (s+\omega^*)^{1-\alpha}\mathcal{L}_t\left\{\exp\left(\omega^* t\right)\rho(t); s+\omega^*\right\} \\
&= (s+\omega^*)^{1-\alpha}\mathcal{L}_t\left\{\rho(t); s\right\} \\
&= \mathcal{L}_t\left\{\rho(t)\right\}\left((\omega^*)^{1-\alpha} + (1-\alpha)(\omega^*)^{-\alpha}s + \mathcal{O}(s^2)\right).
\end{aligned} \tag{3.53}$$

This equation can be inverted term-by-term due to the linearity of the Laplace transform. Hence we find

$$\exp\left(-\omega^* t\right)\, {}_0\mathcal{D}_t^{1-\alpha}\left(\exp\left(\omega^* t\right)\rho(t)\right) = (\omega^*)^{1-\alpha}\rho(t) + (1-\alpha)(\omega^*)^{-\alpha}\frac{\mathrm{d}\rho}{\mathrm{d}t} + \mathcal{L}_s^{-1}\left\{\mathcal{O}(s^2)\right\}. \tag{3.54}$$

Thus in the limit we find

$$\lim_{t\to\infty} \exp\left(-\omega^* t\right)\, {}_0\mathcal{D}_t^{1-\alpha}\left(\exp\left(\omega^* t\right)\rho(t)\right) = (\omega^*)^{1-\alpha}\rho^*. \tag{3.55}$$

Note that this is the same result as simply substituting a constant ρ^* in to the original expression, the key point that we have demonstrated being that the non-locality of the fractional derivative is not unduly affected by pre-asymptotic behaviour. Substituting Eq. (3.55) in to Eq. (3.52) and taking the limit gives,

$$\rho^* = \frac{q^*}{\omega^* + \tau^{-\alpha}\left(\omega^*\right)^{1-\alpha}}\,. \tag{3.56}$$

Analysis of the stability of the equilibrium points is possible, however this is difficult in a general setting. The specific example of a fractional-order SIR model has previously been considered [21].

3.3 Fractional-order Multiple Compartment Model

In general, any number of fractional-order single compartment models can be composed together to form a fractional-order multiple compartment model. The exact nature of how the compartments are joined is system dependent. Consider a set of N compartments, the dynamics of each compartment will be governed by a governing equation of the form,

$$\frac{\mathrm{d}\rho_k}{\mathrm{d}t} = q_k^+(t) - \omega_k(t)\rho_k(t) - \tau_k^{-\alpha_k}\Theta_k(t,0)\,{}_0\mathcal{D}_t^{1-\alpha_k}\left(\frac{\rho_k(t)}{\Theta_k(t,0)}\right), \tag{3.57}$$

where $k = 1, \ldots, N$ indicates the compartment.

In a multiple compartment model the flux entering a compartment, $q_k(t)$, may be dependent on the flux leaving another compartment. This is achieved by matching removal processes from a compartment to creation processes in another. It is also possible to have creation processes that do not depend on removal processes from

other compartments. The Markovian rates, $\omega_k(t)$, are general functions of time and hence may depend on the population in any compartment.

Using this approach we can build the governing equations for any given compartment model, with fractional dynamics. Further demonstration is best done by way of examples and reductions to existing models.

3.4 Examples of Fractional-order Compartment Models

The general framework which we have established in this Chapter can be used to create specific examples of fractional-order compartment models. With the appropriate choice of fluxes, rates, and fractional parameters the general governing equation reduces to the fractional recovery SIR model [21]. We provide fractional models for epidemiological, pharmacokinetic and in-host disease dynamics, with figures demonstrating the fluxes between compartments. In these figures we have defined Markovian transitions with a regular arrow and anomalous transitions with a dashed arrow.

3.4.1 An SIS model with Fractional Re-susceptibility

Similar to the fractional recovery SIR model, a fractional SIS model is a generalisation of the standard SIS model. This model splits the population into a susceptible compartment, S, and an infected compartment I. Individuals start in the susceptible compartment, then transition into the infected compartment through a mass action term, as in the SIR model. Subsequently, individuals undergo an anomalous transition back into the susceptible compartment, as represented in Fig. 3.1.

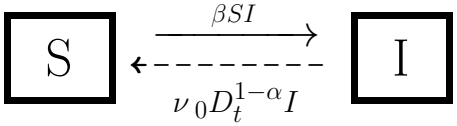

Figure 3.1: Flux flow of fractional SIS Model

We obtain this model from Eq. (3.57). Here, we have two compartments, $\rho_1 = S$ and $\rho_2 = I$. We take the flux into the infected compartment to be $q_2^+(t) = \beta SI$. There is no Markovian removal process from the infected compartment, so that $\omega_2(t) = 0$, and, using Eq. (3.2), $\Theta(t, 0) = 1$. In the fractional SIS model we are considering an anomalous re-susceptibility, we define $\alpha_2 = \alpha$ and $\tau_2^{-\alpha} = \nu$. This yields the governing evolution equation for the infected compartment,

$$\frac{dI}{dt} = \beta SI - \nu\, {}_0\mathcal{D}_t^{1-\alpha}\left(I\right). \tag{3.58}$$

Taking, $q_1^+(t) = \nu\, {}_0\mathcal{D}_t^{1-\alpha}\left(I\right)$, $\omega_1 = \beta S$ and, as there is no non-Markovian removal process, i.e. $\Phi_1(t) = 1$, we can define the governing equation for the susceptible compartment,

$$\frac{dS}{dt} = -\beta SI + \nu\, {}_0\mathcal{D}_t^{1-\alpha}\left(I\right). \tag{3.59}$$

There are no vital dynamics in this model so that the total population is constant for all time, and $S(t)+I(t) = N$, where N is the total population. Equations (3.58) and (3.59), subject to the initial conditions $S(0) = s_0$ and $I(0) = i_0$, define the complete dynamics of the fractional SIS model. While we have constructed this model as an epidemic model, the standard SIS model has been used for general applications such as changing opinion dynamics [149] and it is feasible that the fractional SIS model could be used in a similar way where the time spent in a state affects the probability of switching states.

3.4.2 A Compartment Model for Chromium Clearance in Mice

A fractional-order compartment model can be used to model the clearance of chromium in mice. When chromium enters the body a variety of processes may cause it to become trapped. This includes chemical reactions and the physical trapping of chromium within red blood cells [78]. We can use Eq. (3.46) to model the whole-body clearance of chromium in mice. In this model we consider a single compartment

model which represents the concentration of chromium remaining in the cell, see Fig. 3.2.

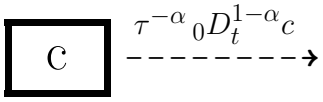

Figure 3.2: Flux flow of chromium clearance

In this example, $\rho = c$ and we consider the only flux into the compartment to occur as an initial dose, i.e. $i_0 = c_0$ and $q^+(t) = 0$. We assume that there are no Markovian removal processes, hence $\omega(t) = 0$ which yields the equation,

$$\frac{dc}{dt} = -\tau^{-\alpha}{}_0\mathcal{D}_t^{1-\alpha}\left(c\left(t\right)\right), \tag{3.60}$$

where $c(0) = c_0$.

We can solve Eq. (3.60), as we did in Eq. (3.62), to give us the solution for the chromium content in the mouse body over time, hence,

$$c(t) = c_0 E_{\alpha,1}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right). \tag{3.61}$$

We compare this model to the experiment by Bryson and Goodall [33], in which the whole-body chromium clearance of mice is observed over time. In this experiment, a high dose of Cr(VI), as potassium dichromate, is injected into a cohort of mice at time, $t = 0$. Mice were sacrificed at three, seven and twenty one days after the initial dose and the total whole body chromium concentration was measured. The experimental results reveal that whole-body clearance of chromium from mice is observed to be rapid during the first week, with 31% of the initial dose remaining after three days and 16% after seven days. Clearance then slows dramatically, at 21 days 7.5% of the initial dose remains [33]. Using a least squares fit we found the best parameters for the Mittag-Leffler solution in Eq. (3.61) to be $\alpha = 0.71$ and

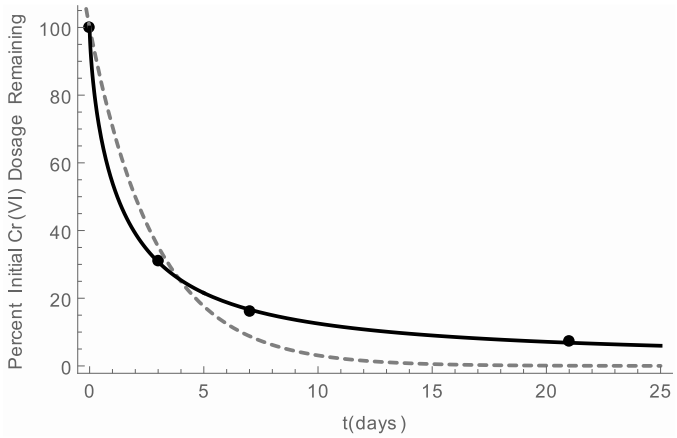

Figure 3.3: Percentage of initial Chromium dose remaining in mice after a time (dots). The ODE single compartment prediction (dashed) and fractional-order single compartment prediction (full).

$\tau = 1.60$. We compare this fit to the solution of a standard constant-decay ODE model for which the solution is an exponential function, $c(t) = c_0 \exp(-t/\tau)$, i.e. $\alpha = 1$. Plots of the solutions are shown in Figure 3.3. The Mittag-Leffler solution shows excellent agreement with the experimental data.

3.4.3 A Compartment Model for in Vivo Dynamics of HIV

Many mathematical models have been developed to study HIV infection and drug treatment in vivo, and the response of the immune system to the infection. These models are typically concerned with modelling the population of CD4+ T cells, the primary target of HIV, and the population of the virus itself [118].

Here we present a simplistic two-compartment model for the population dynamics of the virus and infected CD4+ T-cells. We consider the case of combined antiretroviral therapy with 100% efficacy, meaning there will be no replenishment of the infected T-cells from uninfected stock. We let I denote the number of infected CD4+ T cells and V the number of HIV virions. Virions from Long-lived infected cells are typically observed after treatment has begun [117]. To model this we will have a fractional death of infected cells using Eq. (3.57) with $\rho_1(t) = I(t)$ and $\rho_2(t) = V(t)$, see Fig. 3.4.

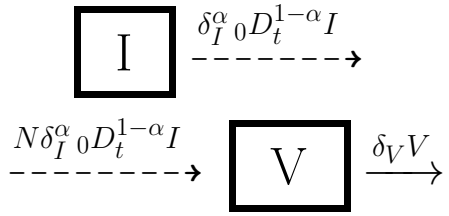

Figure 3.4: Flux flow of fractional HIV model

As no new infected cells are created, $q_1^+(t) = 0$ and the only flux into the infected compartment occurs as the initial conditions, we assume there is no Markovian removal process of infected cells hence, $\omega_1(t) = 0$. We take $\alpha_1 = \alpha$ and $\tau_1 = 1/\delta_I$. This gives us the governing equation for infected cells,

$$\frac{dI}{dt} = -\delta_I^\alpha\,{}_0\mathcal{D}_t^{1-\alpha}I, \tag{3.62}$$

subject to the initial conditions $I(0) = i_0$. Upon death of an infected cell, virions are released. This occurs through a burst event and we will assume that on average N virions are created from each infected cell death. As such we take $q_2^+(t) = N\delta_I^\alpha\,{}_0\mathcal{D}_t^{1-\alpha}I$, and assuming no long lived virions, we will only consider a Markovian death rate of virions. Hence, $\omega_2(t) = \delta_V$, i.e. the governing evolution equation for the number of virions is,

$$\frac{\mathrm{d}V}{\mathrm{d}t} = N\delta_I^\alpha\,{}_0\mathcal{D}_t^{1-\alpha}I - \delta_V V\,, \tag{3.63}$$

subject to the initial conditions $V(0) = V_0$.

The well-known solution [121] of Eq. (3.62) is,

$$I(t) = I_0 E_{\alpha,1}\left(-(\delta_I t)^\alpha\right). \tag{3.64}$$

Substituting Eq. (3.64) into Eq. (3.63) we can then use an integrating factor method to solve for $V(t)$,

$$V(t) = e^{-\delta_V t} I_0 N \left(\left[1 - e^{\delta_V t} E_{\alpha,1} \left(-(\delta_I t)^\alpha \right) \right] + \delta_V \int_0^t e^{\delta_V s} E_{\alpha,1} \left(-(\delta_I s)^\alpha \right) \, \mathrm{d}s \right) + V_0 e^{-\delta_V t}. \tag{3.65}$$

3.5 Summary

We have derived the governing evolution equations for compartment model dynamics from the stochastic process of particles undergoing a CTRW. The resulting dynamics are represented by a coupled set of master equations, Eq. (3.57), derived through Sections 3.2 and 3.3. Under a natural, power-law, choice of waiting time probabilities these master equations become coupled ODEs with fractional dynamics, as demonstrated in Section 3.2.3.

The use of fractional derivatives in compartment models has attracted increasing levels of interest in recent years. It is easy to construct fractional-order compartment models by including fractional derivatives in an *ad hoc* manner, e.g., simply replacing integer order derivatives with fractional-order derivatives. The approach for developing fractional-order compartment models in this thesis starts by considering an underlying stochastic process and fractional-order evolution equations are obtained systematically by considering power-law distributed waiting times in compartments. The *ad hoc* inclusion of fractional derivatives in compartment models can result in equations that are unphysical; they may violate conservation of mass. In Eq. (3.57) we observe an entanglement of the Markovian removal waiting times in the non-Markovian removal processes. This ensures a conservation of probability or mass between the local operators and the non-local fractional derivative operator. Furthermore, in a given physical system, it is to be expected that only some reactions will experience trapping or power-law waiting time. Our derivation accommodates this.

Finally we have provided some simple examples of fractional-order multi-compartment models whose governing evolution equations have been obtained using the methods of this chapter, which will be considered in their discretised form in Chapter 7.

Chapter 4

Fractional Infectivity SIR

4.1 Introduction

The results of this Chapter are drawn from [20]. The main objective in this Chapter is to provide a sound derivation of an SIR model that includes a fractional-order derivative as the infectivity term. Part of the motivation is that some of the *ad hoc* fractional compartment models have been shown to be unphysical [43]. In the case of the fractional-order infectivity SIR model derived here, the fractional derivatives appear if the infectivity of an individual depends on their age-since-infection in a power-law manner. The power-law in the infectivity can arise, as a special case, in a disease process where the longer that a person has been infected, the less likely they are to transmit the disease. The assumptions that give rise to the fractional derivative can be experimentally validated from epidemiological studies by estimating the infectivity as a function of time and time since infection.

The conditions under which the fractional infectivity SIR model occurs, differ to the conditions of the fractional recovery SIR, derived in Chapter 2. In Section 4.2 we derive a general infectivity SIR model from a CTRW and show the consistency of the derived model with a Kermack-McKendrick age-structured SIR model. A power-law rate is considered for the infectivity in Section 4.3. This results in the inclusion of a fractional-order derivative in the infectivity term of the model. The equilibrium states of the system are found in Section 4.4.

4.2 Derivation

In order to incorporate the fractional-order infectivity, we first derive master equations for an SIR model with a general infectivity rate, using a stochastic process. We consider a generalised CTRW where an individual transitions through the three compartments, waiting a random time in each compartment. The model considers an ensemble of such individuals. An individual who has been infectious since time t' will infect a particular susceptible person in the time interval t to $t + \delta t$, with probability $\sigma(t, t')\delta t + o(\delta t)$. The transmission rate per infected individual, $\sigma(t, t')$ is dependent on both the time of infection, t', and current time, t. Given that there are $S(t)$ susceptible people at time t then in the time interval t to $t+\delta t$ the expected number of new infections per infected individual will be $\sigma(t, t')S(t)\delta t + o(\delta t)$.

The number of individuals entering the infected compartment at time t, i.e. the flux into I, will be represented as $q^+(I, t)$. This can be recursively constructed from the flux at earlier times by,

$$q^+(I, t) = \int_{-\infty}^{t} \sigma(t, t')S(t)\Phi(t, t')q^+(I, t')dt', \tag{4.1}$$

where $\Phi(t, t')$ is the survival function that an individual infected at a prior time t' remains infected at time t. Considering the initial distribution of infected individuals in the population, we let $i(-t', 0)$ be the number of individuals who became infected at time $t' < 0$ and who are still infected at time 0, hence,

$$q^+(I, t') = \frac{i(-t', 0)}{\Phi(0, t')}, \quad t' < 0. \tag{4.2}$$

Hence we can split Eq. (4.1) into,

$$q^+(I, t) = \int_{0}^{t} \sigma(t, t')S(t)\Phi(t, t')q^+(I, t')dt' + \int_{-\infty}^{0} \sigma(t, t')S(t)\frac{\Phi(t, t')}{\Phi(0, t')}i(-t', 0)dt'. \tag{4.3}$$

It is natural to assume that the rate of infection, $\sigma(t, t')$, is dependent on the time t to account for environmental changes in time. It is expected that $\sigma(t, t')$ may also depend on the age of infection, $t - t'$, to account for the natural course of the disease. In the following we incorporate these effects by writing,

$$\sigma(t, t') = \omega(t)\rho(t - t'). \tag{4.4}$$

Noting that an individual may leave the infected compartment in two ways, either they die or they recover from the disease, and assuming these effects are independent we can write the survival function as,

$$\Phi(t, t') = \phi(t, t')\theta(t, t'). \tag{4.5}$$

Here $\phi(t, t')$ is the probability of surviving the transition to the R compartment from time t' to time t, and $\theta(t, t')$ is the probability of surviving the death transition from time t' until time t. We will assume that the recovery and death survival take the form,

$$\theta(t, t') = e^{-\int_{t'}^{t} \gamma(s)ds}, \tag{4.6}$$

$$\phi(t, t') = e^{-\int_{t'}^{t} \mu(s)ds}. \tag{4.7}$$

From this it follows that $\Phi(t, t')$ satisfies the semi-group property,

$$\Phi(t, t') = \Phi(t, s)\Phi(s, t'), \quad \forall\, t' < s < t. \tag{4.8}$$

For an individual to be infected at time t they must have become infected at some time prior to t and not yet transitioned into the removed compartment nor died. Hence the number of individuals in the I compartment at time t can be expressed

recursively using the flux as,

$$I(t) = I_0(t) + \int_0^t \Phi(t,t')q^+(I,t')dt'. \tag{4.9}$$

In Eq. (4.9) $I_0(t)$ is the number of initially infected individuals, $i(-t',0)$, whose infection has persisted until time t, expressed as,

$$\begin{aligned} I_0(t) &= \int_{-\infty}^0 \frac{\Phi(t,t')}{\Phi(0,t')} i(-t',0)dt', \\ &= \Phi(t,0)\int_{-\infty}^0 i(-t',0)dt'. \end{aligned} \tag{4.10}$$

In order to recover the master equations governing the dynamics, we differentiate Eq. (4.9) to produce,

$$\begin{aligned} \frac{dI(t)}{dt} &= q^+(I,t) - (\mu(t)+\gamma(t))\int_0^t \phi(t,t')\theta(t,t')q^+(I,t')dt' - (\gamma(t)+\mu(t))I_0(t), \\ &= q^+(I,t) - (\mu(t)+\gamma(t))I(t). \end{aligned} \tag{4.11}$$

Substituting Eqs. (4.3), (4.4) into Eq. (4.11) gives,

$$\begin{aligned} \frac{dI(t)}{dt} = &\int_0^t \omega(t)\rho(t-t')S(t)\Phi(t,t')q^+(I,t')dt' + \int_{-\infty}^0 \omega(t)\rho(t-t')S(t)\Phi(t,0)i(-t',0)dt' \\ &- (\mu(t)+\gamma(t))I(t). \end{aligned} \tag{4.12}$$

In order to obtain a generalised master equation we need to express the right hand side of this equation in terms of $I(t)$. We can write Eq. (4.9) using Eq. (4.8) as,

$$\frac{I(t)}{\Phi(t,0)} = \frac{I_0(t)}{\Phi(t,0)} + \int_0^t \frac{q^+(I,t')}{\Phi(t',0)}dt'. \tag{4.13}$$

Taking the Laplace transform from t to s then gives,

$$\mathcal{L}\left\{\frac{q^+(I,t)}{\Phi(t,0)}\right\} = s\mathcal{L}\left\{\frac{I(t)-I_0(t)}{\Phi(t,0)}\right\}. \tag{4.14}$$

Returning to the first integral of Eq. (4.12) we can rewrite it using Laplace transforms as,

$$\omega(t)S(t)\int_0^t \rho(t-t')\frac{q^+(I,t')}{\Phi(t',0)}dt' = \omega(t)S(t)\mathcal{L}^{-1}\left\{\mathcal{L}\{\rho(t)\}\mathcal{L}\left\{\frac{q^+(I,t)}{\Phi(t,0)}\right\}\right\}. \tag{4.15}$$

Making use of Eq. (4.14) this becomes,

$$\begin{aligned}\omega(t)S(t)\mathcal{L}^{-1}\left\{\mathcal{L}\{\rho(t)\}\mathcal{L}\left\{\frac{q^+(I,t)}{\Phi(t,0)}\right\}\right\} &= \omega(t)S(t)\mathcal{L}^{-1}\left\{s\mathcal{L}\{\rho(t)\}\mathcal{L}\left\{\frac{I(t)-I_0(t)}{\Phi(t,0)}\right\}\right\},\\ &= \omega(t)S(t)\int_0^t \kappa(t-t')\frac{I(t')-I_0(t')}{\Phi(t',0)}dt',\end{aligned} \tag{4.16}$$

where we have defined,

$$\kappa(t) = \mathcal{L}^{-1}\{s\mathcal{L}\{\rho(t)\}\}. \tag{4.17}$$

Using Eqs. (4.16) and (4.17), in Eq. (4.12), we obtain the master equation,

$$\begin{aligned}\frac{dI(t)}{dt} =&\omega(t)S(t)\Phi(t,0)\left(\int_0^t \kappa(t-t')\frac{I(t')-I_0(t')}{\Phi(t',0)}dt' + \int_{-\infty}^0 \rho(t-t')i(-t',0)dt'\right)\\ &- \mu(t)I(t) - \gamma(t)I(t).\end{aligned} \tag{4.18}$$

Noting that $\frac{I_0(t)}{\Phi(t,0)}$ is a constant and using Eq. (4.17) this may be written as,

$$\begin{aligned}\frac{dI(t)}{dt} =&\omega(t)S(t)\Phi(t,0)\left(\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt' + \int_{-\infty}^0 \left(\rho(t-t')-\rho(t)\right)i(-t',0)dt'\right)\\ &- \mu(t)I(t) - \gamma(t)I(t).\end{aligned} \tag{4.19}$$

This equation is the generalised master equation that describes the time evolution of the number of infected individuals in an SIR model with arbitrary time dependent infectivity and recovery. As individuals may only enter the infected compartment from the susceptible compartment, there must be a corresponding decrease in the number of individuals in the susceptible compartment. Accounting for vital dynamics, the differential equation for the susceptible population is then given by,

$$\begin{aligned}\frac{dS(t)}{dt} =&\lambda(t) - \omega(t)S(t)\Phi(t,0)\left(\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt'\right.\\ &\left.+\int_{-\infty}^0 (\rho(t-t')-\rho(t))i(-t',0)dt'\right) - \gamma(t)S(t),\end{aligned} \tag{4.20}$$

where $\lambda(t) \geq 0$ is the birth rate and $\gamma(t) \geq 0$ is the per capita death rate. Using a similar balance between the infected and recovered compartment, the differential equation for the recovered compartment is,

$$\frac{dR(t)}{dt} = \mu(t)I(t) - \gamma(t)R(t). \tag{4.21}$$

Taking the initial condition $i(-t,0) = i_0\delta(-t)$, where $\delta(-t)$ is a Dirac delta function and i_0 is a constant, these equations further simplify to give,

$$\frac{dS(t)}{dt} =\lambda(t) - \omega(t)S(t)\Phi(t,0)\left(\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt'\right) - \gamma(t)S(t), \tag{4.22}$$

$$\frac{dI(t)}{dt} =\omega(t)S(t)\Phi(t,0)\left(\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt'\right) - \mu(t)I(t) - \gamma(t)I(t), \tag{4.23}$$

$$\frac{dR(t)}{dt} =\mu(t)I(t) - \gamma(t)R(t). \tag{4.24}$$

4.2.1 Structured SIR

Here we show how the master equations, Eqs. (4.22), (4.23), (4.24), can be reduced to the Kermack and McKendrick age-structured SIR model [74] equations given by,

$$\begin{aligned}
\frac{dS}{dt} &= \lambda - S(t)\int_0^\infty \nu(t,a)i(a,t)da - \gamma S(t), && (4.25)\\
\frac{\partial i}{\partial t} &+ \frac{\partial i}{\partial a} = -\beta(a)i(a,t) - \gamma i(a,t), && (4.26)\\
\frac{dR}{dt} &= \int_0^\infty \beta(a)i(a,t)da - \gamma R(t), && (4.27)\\
I(t) &= \int_0^\infty i(a,t)da. && (4.28)
\end{aligned}$$

In this model we consider $i(a,t)$ to be the number of the individuals infected at time t who have been infected for length of time a. To show how Eq. (4.23) reduces to Eq. (4.26) we set $i(a,t)$ to,

$$i(a,t) = \Phi(t,t-a)q^+(I,t-a). \tag{4.29}$$

This allows us to see that $i(0,t) = q^+(I,t)$. Integrating Eq. (4.26) with respect to a, using Eq. (4.28) and equating $\beta(a) = \mu$ yields,

$$\frac{dI(t)}{dt} = q^+(I,t) - \mu\int_0^\infty \Phi(t,t-a)q^+(I,t-a)da - \gamma I(t). \tag{4.30}$$

By taking a change in variable to $t' = t - a$ and making use of Eqs. (4.3) and (4.4) we arrive at,

$$\begin{aligned}
\frac{dI(t)}{dt} &= \int_0^t \rho(t-t')\omega(t)S(t)\Phi(t,t')q^+(I,t')dt' \\
&+ \int_{-\infty}^0 \rho(t-t')\omega(t)S(t)\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt' - \mu\int_{-\infty}^t \Phi(t,t')q^+(I,t')dt' - \gamma I(t).
\end{aligned} \tag{4.31}$$

We further simplify this expression by using Eqs. (4.14), (4.15) and (4.16) and taking the initial condition to be $i(-t', 0) = i_0\delta(-t')$. This yields,

$$\frac{dI(t)}{dt} = \omega(t)S(t)\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt' - \mu I(t) - \gamma I(t), \tag{4.32}$$

which is a special case of Eq. (4.23). To show how Eq. (4.22) reduces to Eq. (4.25) we consider a change of variable $a = t - t'$, hence we can rewrite Eq. (4.25) as,

$$\frac{dS(t)}{dt} = \lambda - S(t)\int_{-\infty}^t \nu(t, t-t')\Phi(t,t')q^+(I,t')dt' - \gamma S(t), \tag{4.33}$$

which is equivalent to Eq. (4.22) if $\nu(t, t-t') = \sigma(t, t')$. Finally to recover Eq. (4.24) from Eq. (4.27) we make use of Eq. (4.29) and the change of variable $a = t - t'$, resulting in,

$$\frac{dR(t)}{dt} = \mu I(t) - \gamma R(t). \tag{4.34}$$

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The general master equations given in Eqs. (4.22), (4.23), (4.24) reduce to the classic SIR ODEs if $\rho(t) = \rho$, a constant. This can be seen from Eq. (4.17) where the corresponding memory kernel reduces to,

$$\kappa(t) = \rho\delta(t). \tag{4.35}$$

If $\rho(t)$ is a power-law of the form,

$$\rho(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}, \quad 0 < \alpha \leq 1, \tag{4.36}$$

then the general master equations reduce to a set of fractional-order differential equations. The memory kernel following from Eq. (4.17) with power-law $\rho(t)$ given

by Eq. (4.17) has Laplace transform,

$$\mathcal{L}_t\{\kappa(t)\} = s^{1-\alpha}. \tag{4.37}$$

Hence the integral in Eqs. (4.22) and (4.23) can be written as follows,

$$\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt' = \int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t,0)}dt', \tag{4.38}$$

$$= \mathcal{L}_s^{-1}\left\{s^{1-\alpha}\mathcal{L}_t\left\{\frac{I(t')}{\Phi(t',0)}\right\}\right\}. \tag{4.39}$$

To evaluate the inverse Laplace transform in the above equation we use Eq. (1.9), ${}_0\mathcal{D}_t^{-\alpha}f(t)\big|_{t=0^+} = 0$, and we can express Eq. (4.38) as,

$$\int_0^t \kappa(t-t')\frac{I(t')}{\Phi(t',0)}dt' = {}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t')}{\Phi(t',0)}\right). \tag{4.40}$$

Substituting Eq. (4.40) into the generalised master equations Eqs. (4.22) and (4.23) yields the fractional-order infectivity SIR model,

$$\frac{dS(t)}{dt} = \lambda(t) - \omega(t)S(t)\Phi(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\Phi(t,0)}\right) - \gamma(t)S(t), \tag{4.41}$$

$$\frac{dI(t)}{dt} = \omega(t)S(t)\Phi(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\Phi(t,0)}\right) - \mu(t)I(t) - \gamma(t)I(t), \tag{4.42}$$

$$\frac{dR(t)}{dt} = \mu(t)I(t) - \gamma(t)R(t). \tag{4.43}$$

4.3.1 Dimensionality

An aspect of fractional SIR models that warrants further consideration is the dimensionality of the parameters. A time derivative of order one has dimension of $[\text{time}]^{-1}$, a fractional derivative of order α, either a Caputo or Riemann-Liouville, will have a dimension of $[\text{time}]^{-\alpha}$. Hence the inclusion of fractional derivatives necessitates the redefinition of parameters in the associated models. This may lead to complications when considering the physical interpretation of rates [43].

In the fractional model derived above, we consider the equation for change in the number of infected individuals over time, Eq. (4.42). As we have a order one time derivative of a population on the left hand side its dimension is [population][time]$^{-1}$. Thus the dimension of the right hand side must be the same. It is clear that the recovery and death rates, $\mu(t)$, and $\gamma(t)$, must have dimension [time]$^{-1}$ as $I(t)$ has the dimension [population].

For the infectivity term, it is clear that the dimension of $S(t)$ is [population], and the fractional derivative ${}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\Phi(t,0)}\right)$ is [population][time]$^{\alpha-1}$. In order for the dimensions of the infectivity term to be consistent with the model, we are left with $\omega(t)$ having dimension [population]$^{-1}$[time]$^{-\alpha}$. We note that the dimensions of the infectivity rate per infected individual of the disease, $\sigma(t,t') = \omega(t)\rho(t-t')$, is [population]$^{-1}$[time]$^{-1}$, regardless of the fractional α exponent.

4.4 Equilibrium State Analysis

The set of fractional infectivity SIR Eqs. (4.41), (4.42) and (4.43) are a non-autonomous dynamical system. This set up creates difficulty in finding the equilibrium states hence we will simplify the model by taking the birth, death, recovery and contact rates to be constant, i.e. $\lambda(t) = \lambda$, $\gamma(t) = \gamma$, $\mu(t) = \mu$ and $\omega(t) = \omega_\alpha$ respectively, where ω_α represents the dependence of the chosen α exponent on $\omega(t)$, due to dimensionality considerations. Hence the model becomes,

$$\frac{dS(t)}{dt} = \lambda - \omega_\alpha S(t)\Phi(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\Phi(t,0)}\right) - \gamma S(t), \tag{4.44}$$

$$\frac{dI(t)}{dt} = \omega_\alpha S(t)\Phi(t,0)\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\Phi(t,0)}\right) - \mu I(t) - \gamma I(t), \tag{4.45}$$

$$\frac{dR(t)}{dt} = \mu I(t) - \gamma R(t). \tag{4.46}$$

This can be simplified further using Eqs. (4.5), (4.6), (4.7) to rewrite,

$$\Phi(t,0) = e^{-(\gamma+\mu)t}. \tag{4.47}$$

The equilibrium state, (S^*, I^*, R^*), is defined by,

$$\lim_{t\to\infty} S(t) = S^*, \qquad \lim_{t\to\infty} I(t) = I^*, \qquad \lim_{t\to\infty} R(t) = R^*.$$

Taking the limit as $t \to \infty$ of Eqs. (4.44), (4.45) and (4.46) reduces the equations to,

$$0 = \lambda - \lim_{t\to\infty} \omega_\alpha S(t) e^{-(\gamma+\mu)t}\, {}_0\mathcal{D}_t^{1-\alpha} \left(e^{(\gamma+\mu)t} I(t)\right) - \gamma S^*, \tag{4.48}$$

$$0 = \lim_{t\to\infty} \omega_\alpha S(t) e^{-(\gamma+\mu)t}\, {}_0\mathcal{D}_t^{1-\alpha} \left(e^{(\gamma+\mu)t} I(t)\right) - (\gamma+\mu) I^*, \tag{4.49}$$

$$0 = \mu I^* - \gamma R^*. \tag{4.50}$$

We are able to split the remaining limit into,

$$\lim_{t\to\infty} \omega_\alpha S(t) e^{-\nu t}\, {}_0\mathcal{D}_t^{1-\alpha} \left(e^{\nu t} I(t)\right) = \left(\lim_{t\to\infty} \omega_\alpha S(t)\right) \left(\lim_{t\to\infty} e^{-\nu t}\, {}_0\mathcal{D}_t^{1-\alpha} \left(e^{\nu t} I(t)\right)\right),$$

where $\nu = \gamma + \mu$. Using the result of [21],

$$\lim_{t\to\infty} e^{-\nu t}\, {}_0\mathcal{D}_t^{1-\alpha} \left(e^{\nu t} I(t)\right) = \nu^{1-\alpha} I^*,$$

and trivially we have $\lim_{t\to\infty} \omega_\alpha S(t) = \omega_\alpha S^*$, hence,

$$\lim_{t\to\infty} \omega_\alpha S(t) e^{-\nu t}\, {}_0\mathcal{D}_t^{1-\alpha} \left(e^{\nu t} I(t)\right) = \omega_\alpha (\gamma+\mu)^{1-\alpha} S^* I^*. \tag{4.51}$$

Substituting Eq. (4.51) into Eqs. (4.48), (4.49) and (4.50) yields,

$$0 = \lambda - \omega_\alpha (\mu+\gamma)^{1-\alpha} S^* I^* - \gamma S^*, \tag{4.52}$$

$$0 = \omega_\alpha (\mu+\gamma)^{1-\alpha} S^* I^* - (\mu+\gamma) I^*, \tag{4.53}$$

$$0 = \mu I^* - \gamma R^*. \tag{4.54}$$

Solving these equations reveals two equilibrium states, the disease free state,

$$S^* = \frac{\lambda}{\gamma}, \quad I^* = 0, \quad R^* = 0, \tag{4.55}$$

and the endemic state,

$$S^* = \frac{\mu+\gamma}{\omega_\alpha(\mu+\gamma)^{1-\alpha}}, \quad I^* = \frac{\lambda}{\mu+\gamma} - \frac{\gamma}{\omega_\alpha(\mu+\gamma)^{1-\alpha}}, \quad R^* = \frac{\mu}{\gamma}\left(\frac{\lambda}{\mu+\gamma} - \frac{\gamma}{\omega_\alpha(\mu+\gamma)^{1-\alpha}}\right). \tag{4.56}$$

The disease free equilibrium state is non-negative for all valid system parameters. However, the endemic equilibrium is only non-negative if,

$$\frac{\lambda\omega_\alpha}{\gamma} > (\mu+\gamma)^\alpha. \tag{4.57}$$

In the case where $\alpha = 1$ the equilibrium states reduce to the steady states of the standard SIR ODE model with vital dynamics. We anticipate that, similar to the fractional recovery SIR model [21], the endemic equilibrium state will be an asymptotically stable state for all parameters where it is non-negative.

4.4.1 Basic Reproduction Number

A fundamental quantity of interest in SIR models is the basic reproduction number R_0 defined as the number of new infections that an infected person will produce over the course of their infection in an otherwise uninfected population. This can be calculated from

$$R_0 = N\int_0^\infty \omega_\alpha \rho(t')\Phi(t',0)\,dt' \tag{4.58}$$

where N is the total population. After substituting Eq. (4.36), and Eq. (4.47), into the above we obtain the result,

$$R_0 = \frac{\omega_\alpha N}{(\gamma+\mu)^\alpha}. \tag{4.59}$$

This defines the basic reproduction number for fractional infectivity SIR model. Given that the equilibrium population is given by,

$$\begin{aligned} N =& \lim_{t\to\infty} S(t) + I(t) + R(t) \\ =& \frac{\lambda}{\gamma}, \end{aligned} \tag{4.60}$$

it then follows from Eq. (4.57) that the existence of the endemic equilibrium requires $R_0 > 1$. It is worth noting that the integral in Eq. (4.58) would diverge for $\rho(t) \sim t^{-\beta}$ with $\beta > 1$, which is consistent with the restriction $0 < \alpha \leq 1$ in Eq. (4.36).

4.5 Summary

In this Chapter, we have provided a physical derivation of an SIR model that includes fractional-order derivatives. This is motivated by the concerns that many fractional-order compartment models that have been postulated are not physically meaningful. Starting from a stochastic process, we have derived an SIR model where the evolution equations incorporate a fractional-order derivative in the infectivity term. This derivative arises from a power-law dependence in the infectivity. We have shown that this fractional infectivity SIR model can be written as an age structured SIR model. The dimensions of the parameters in the fractional model depend on the order of the fractional derivative. The fractional model permits both a disease free, and an endemic, long time equilibrium state, dependent on the system parameters. Whilst we have not identified a particular disease process with the required power-law properties of the infectivity that gives rise to the fractional derivatives in the model these assumptions could be experimentally validated from epidemiological studies by estimating the infectivity $\sigma(t, t')$ as a function of time t, and time of infection t'.

Chapter 5

Fractional Infectivity and Fractional Recovery SIR

5.1 Introduction

In this Chapter we extend the stochastic process derivation of an SIR model considered in the past three chapters to allow for a fractional infectivity and fractional recovery. This Chapter follows the publication [22]. In Section 5.2 we derive the governing master equations of an SIR model from a stochastic process with general history dependent infectivity and recovery. In Section 5.3 we consider particular forms of the infectivity and recovery such that the governing equations will contain fractional derivatives. In Section 5.4 we consider the limits under which the fractional-order infectivity and recovery SIR model reduce back to the classic and fractional recovery SIR models. In Section 5.5 we derive the steady states of the fractional-order infectivity and recovery SIR model.

5.2 Derivation

We incorporate both a fractional-order infectivity and recovery into an SIR model by deriving the master equations for a stochastic SIR model with age since infection dependences. We consider a generalised CTRW through three compartments, those susceptible (S) to the infection, those infectious (I) with the infection and those recovered (R) from the infection. An individual is born into the S compartment. They wait a random amount of time in each compartment before moving to the next compartment. The individual may die in any compartment and be removed

from consideration. Here we derive the master equations for the time evolution of an ensemble of individuals undergoing these dynamics.

Considering an individual who has been infectious since time t', the probability this infectious individual will infect a particular susceptible person in the time interval t to $t+\delta t$, is $\sigma(t,t')\delta t + o(\delta t)$. The transmission rate per infected individual, $\sigma(t,t')$ is dependent on both how long the individual has been infectious, $t-t'$, and the current time, t. If there are $S(t)$ susceptible individuals at time t then in the time interval t to $t+\delta t$ the expected number of new infections per infected individual will be $\sigma(t,t')S(t)\delta t + o(\delta t)$.

The probability that an individual who is infected at time t' is still infected at time t is given by the survival function $\Phi(t,t')$. For an individual to become infected at time t they must come in contact with an individual who has become infected already. The flux of individuals into the infected compartment, I, at time t, is denoted $q^+(I,t)$, will therefore be constructed recursively via,

$$q^+(I,t) = \int_{-\infty}^{t} \sigma(t,t')S(t)\Phi(t,t')q^+(I,t')dt'. \tag{5.1}$$

Initial conditions are given as the number of individuals who are infected at time 0, and how long each individual has been infected. This is given by the function $i(-t',0)$ that represents the number of individuals that are still infected at time 0 who were originally infected at some earlier time t', hence,

$$q^+(I,t') = \frac{i(-t',0)}{\Phi(0,t')}, \quad t' < 0. \tag{5.2}$$

Equation (5.1) can then be written,

$$q^+(I,t) = \int_{0}^{t} \sigma(t,t')S(t)\Phi(t,t')q^+(I,t')dt' + \int_{-\infty}^{0} \sigma(t,t')S(t)\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt'. \tag{5.3}$$

We will assume that the rate of infection, $\sigma(t, t')$ will be a function of both the current time, t, and the time since infection, $t - t'$. This accounts for both time dependent extrinsic changes as well as the intrinsic change in the infectivity of the disease over its natural course. As such we may write,

$$\sigma(t, t') = \omega(t)\rho(t - t'), \tag{5.4}$$

where $\omega(t) \geq 0$ is the extrinsic infectivity and $\rho(t) \geq 0$ is the intrinsic infectivity. An individual may only leave the infected compartment by either dying or recovering from the disease. Assuming that these processes are independent, the survival function for remaining in the infectious compartment can be written,

$$\Phi(t, t') = \phi(t - t')\theta(t, t'). \tag{5.5}$$

Here $\phi(t-t')$ is the probability that an individual has not recovered and transitioned to the R compartment by time t given that they were infected at an earlier time t'. Similarly $\theta(t, t')$ is the probability that the an individual has not died by time t given that they were infected at the earlier time t'. We will assume that the survival function of the death process takes the form,

$$\theta(t, t') = e^{-\int_{t'}^{t} \gamma(u)du}, \tag{5.6}$$

and hence,

$$\theta(t, t') = \theta(t, u)\theta(u, t'), \ \ \forall\, t' < u < t. \tag{5.7}$$

Individuals in the infected compartment at time t must have arrived in the compartment at some earlier time and not left the compartment. We can therefore express the number of individuals in the infectious compartment via the flux into

the compartment and the survival function to give,

$$I(t) = I_0(t) + \int_0^t \Phi(t,t')q^+(I,t')dt'. \tag{5.8}$$

The function, $I_0(t)$, gives the number of individuals who were infected at time 0, who are still infected at time t. In terms of the initial condition function, $i(-t',0)$, this can be written,

$$I_0(t) = \int_{-\infty}^0 \frac{\Phi(t,t')}{\Phi(0,t')} i(-t',0)dt'. \tag{5.9}$$

The master equations are derived by differentiating Eq. (5.8). This yields,

$$\begin{aligned}\frac{dI(t)}{dt} =& q^+(I,t) - \int_0^t \psi(t-t')\theta(t,t')q^+(I,t')dt' - \gamma(t)\int_0^t \phi(t-t')\theta(t,t')q^+(I,t')dt' \\ &+ \frac{dI_0(t)}{dt},\end{aligned} \tag{5.10}$$

where $\psi(t) = -\frac{d\phi(t)}{dt}$ is the probability density function related to $\phi(t)$. Using Eqs. (5.3), (5.4) and (5.5), Eq. (5.10) can be written,

$$\begin{aligned}\frac{dI(t)}{dt} =& \omega(t)S(t)\left(\int_0^t \rho(t-t')\Phi(t,t')q^+(I,t')dt' + \int_{-\infty}^0 \rho(t-t')\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt'\right) \\ &- \int_0^t \psi(t-t')\theta(t,t')q^+(I,t')dt' + \theta(t,0)\frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right) - \gamma(t)I(t).\end{aligned} \tag{5.11}$$

A generalised master equation can be obtained by removing the dependence on $q^+(I,t)$ in the above equation. Using Eq. (5.7), Eq. (5.8) can be rewritten as,

$$\frac{I(t)}{\theta(t,0)} = \frac{I_0(t)}{\theta(t,0)} + \int_0^t \phi(t-t')\frac{q^+(I,t')}{\theta(t',0)}dt'. \tag{5.12}$$

As this is now in the form of a convolution, taking a Laplace transform from t to s, $\mathcal{L}\{\cdot\}$, then gives,

$$\mathcal{L}\left\{\frac{I(t)-I_0(t)}{\theta(t,0)}\right\} = \mathcal{L}\left\{\phi(t)\right\}\mathcal{L}\left\{\frac{q^+(I,t)}{\theta(t,0)}\right\}. \tag{5.13}$$

Again using Eq. (5.7), the first integral of Eq. (5.11) can be rewritten using Laplace transforms as,

$$\mathcal{L}\left\{\int_0^t \rho(t-t')\phi(t-t')\frac{q^+(I,t')}{\theta(t',0)}dt'\right\} = \mathcal{L}\{\rho(t)\phi(t)\}\mathcal{L}\left\{\frac{q^+(I,t)}{\theta(t,0)}\right\}. \tag{5.14}$$

Making use of Eq. (5.13) this becomes,

$$\begin{aligned}\mathcal{L}\{\rho(t)\phi(t)\}\mathcal{L}\left\{\frac{q^+(I,t)}{\theta(t,0)}\right\} &= \frac{\mathcal{L}\{\rho(t)\phi(t)\}}{\mathcal{L}\left\{\phi(t)\right\}}\mathcal{L}\left\{\frac{I(t)-I_0(t)}{\theta(t,0)}\right\} \\ &= \mathcal{L}\left\{\int_0^t K_I(t-t')\frac{I(t')-I_0(t')}{\theta(t',0)}dt'\right\}.\end{aligned} \tag{5.15}$$

Here we have defined the infectivity memory kernel as,

$$K_I(t) = \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{\rho(t)\phi(t)\}}{\mathcal{L}\{\phi(t)\}}\right\}, \tag{5.16}$$

where $\mathcal{L}^{-1}\{\cdot\}$ defines the inverse Laplace transform from s to t. Once again using Eq. (5.7), the third integral of Eq. (5.11) can similarly be rewritten using Laplace transforms as,

$$\mathcal{L}\left\{\int_0^t \psi(t-t')\frac{q^+(I,t')}{\theta(t',0)}dt'\right\} = \mathcal{L}\{\psi(t)\}\mathcal{L}\left\{\frac{q^+(I,t)}{\theta(t,0)}\right\}. \tag{5.17}$$

Making use of Eq. (5.13) this becomes,

$$\begin{aligned}\mathcal{L}\{\psi(t)\}\mathcal{L}\left\{\frac{q^+(I,t)}{\theta(t,0)}\right\} &= \frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\left\{\phi(t)\right\}}\mathcal{L}\left\{\frac{I(t)-I_0(t)}{\theta(t,0)}\right\} \\ &= \mathcal{L}\left\{\int_0^t K_R(t-t')\frac{I(t')-I_0(t')}{\theta(t',0)}dt'\right\}.\end{aligned} \tag{5.18}$$

Here we have defined the recovery memory kernel,

$$K_R(t) = \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\{\phi(t)\}}\right\}. \tag{5.19}$$

Using Eq. (5.15) and Eq. (5.18), Eq. (5.11) becomes the master equation for the infectious compartment,

$$\begin{aligned}\frac{dI(t)}{dt} =&\omega(t)S(t)\left(\theta(t,0)\int_0^t K_I(t-t')\frac{I(t')-I_0(t')}{\theta(t',0)}dt' + \int_{-\infty}^0 \rho(t-t')\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt'\right)\\ &- \theta(t,0)\left(\int_0^t K_R(t-t')\frac{I(t')-I_0(t')}{\theta(t',0)}dt' - \frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right)\right) - \gamma(t)I(t).\end{aligned} \tag{5.20}$$

This equation governs the time evolution of the number of individuals in the infectious compartment. All individuals who enter the infectious compartment must have previously been susceptible. Taking this into account we may write the master equation for the susceptible compartment, with the addition of the vital dynamics, as

$$\begin{aligned}\frac{dS(t)}{dt} =&\lambda(t) - \omega(t)S(t)\left(\theta(t,0)\int_0^t K_I(t-t')\frac{I(t')-I_0(t')}{\theta(t',0)}dt'\right.\\ &\left.+\int_{-\infty}^0 \rho(t-t')\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt'\right) - \gamma(t)S(t),\end{aligned} \tag{5.21}$$

where $\lambda(t) \geq 0$ is the flux into the compartment due to births. The per capita death rate is assumed to be the same as for the infectious compartment. Similarly considering that individuals who enter the recovered compartment must have left the infectious compartment, we write the master equation for the recovered compartment as,

$$\frac{dR(t)}{dt} = \theta(t,0)\left(\int_0^t K_R(t-t')\frac{I(t')-I_0(t')}{\theta(t',0)}dt' - \frac{d}{dt}\left(\frac{I_0(t)}{\theta(t,0)}\right)\right) - \gamma(t)R(t). \tag{5.22}$$

Together Eqs. (5.21), (5.20) and (5.22) are the master equations for an SIR model with both time since infection dependent infectivity and recovery. These equations are simplified by taking the initial conditions to be $i(-t,0) = i_0\delta(-t)$, where $\delta(t)$ is the Dirac delta function and i_0 is a constant. With these choices we can write,

$$\int_{-\infty}^{0} \rho(t-t')\frac{\Phi(t,t')}{\Phi(0,t')}i(-t',0)dt = \rho(t)i_0\Phi(t,0). \tag{5.23}$$

This leads to simplifications and our full set of SIR master equations become,

$$\frac{dS(t)}{dt} = \lambda(t) - \omega(t)S(t)\theta(t,0)\int_0^t K_I(t-t')\frac{I(t')}{\theta(t',0)}dt' - \gamma(t)S(t), \tag{5.24}$$

$$\frac{dI(t)}{dt} = \omega(t)S(t)\theta(t,0)\int_0^t K_I(t-t')\frac{I(t')}{\theta(t',0)}dt' - \theta(t,0)\int_0^t K_R(t-t')\frac{I(t')}{\theta(t',0)}dt' - \gamma(t)I(t), \tag{5.25}$$

$$\frac{dR(t)}{dt} = \theta(t,0)\int_0^t K_R(t-t')\frac{I(t')}{\theta(t',0)}dt' - \gamma(t)R(t). \tag{5.26}$$

Henceforth we will use the master equations with Dirac delta initial conditions for simplicity.

5.3 Fractional Infectivity and Recovery SIR

We incorporate fractional derivatives into both the infective and recovery terms by choosing $\psi(t)$ to be power-law distributed and $\rho(t)$ related to our choice of $\psi(t)$. Similar to Section 2.3, we take $\psi(t)$ to be Mittag-Leffler distributed,

$$\psi(t) = \frac{t^{\alpha-1}}{\tau^\alpha}E_{\alpha,\alpha}\left(-\left(\frac{t}{\tau}\right)^\alpha\right), \tag{5.27}$$

for $0 < \alpha \leq 1$, where τ is a scaling parameter, and the corresponding survival function $\phi(t)$ is,

$$\phi(t) = E_{\alpha,1}\left(-\left(\frac{t}{\tau}\right)^\alpha\right). \tag{5.28}$$

The Laplace transform of the recovery memory kernel, Eq. (5.19), with Mittag-Leffer distributed $\psi(t)$ is given by,

$$\mathcal{L}\{K_R(t)\} = \frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\{\phi(t)\}} = s^{1-\alpha}\tau^{-\alpha}, \tag{5.29}$$

subsequently, a convolution with the recovery memory kernel can be written as,

$$\int_0^t K_R(t-t')\frac{I(t')}{\theta(t',0)}dt' = \tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right). \tag{5.30}$$

A fractional derivative can be incorporated into the infectivity, if the infective memory kernel, Eq. (5.16), has a Laplace transform similar to Eq. (5.29). This is satisfied by taking $\rho(t)$ of the form,

$$\rho(t) = \frac{1}{\phi(t)}\frac{t^{\beta-1}}{\tau^{\beta}}E_{\alpha,\beta}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right), \tag{5.31}$$

where $\phi(t)$ is defined in Eq. (5.28). As we require $\rho(t) \geq 0$, we must constrain α and β such that $0 < \alpha \leq \beta \leq 1$. This constraint is easily verifiable for $\beta = \alpha$ as $\rho(t)$ can be reduced to,

$$\rho(t) = \frac{1}{\phi(t)}\frac{t^{\alpha-1}}{\tau^{\alpha}}E_{\alpha,\alpha}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right) = \frac{\psi(t)}{\phi(t)}, \tag{5.32}$$

where $\psi(t)$, as defined in Eq. (5.27), and $\phi(t)$ are both positive functions. It is also possible to express Eq. (5.31) using fractional derivatives as,

$$\rho(t) = \frac{\tau^{-\beta}}{\phi(t)}\,{}_0\mathcal{D}_t^{1-\beta}\phi(t). \tag{5.33}$$

Using this form, it is clearer to see that the Laplace transform of the infectivity memory kernel becomes,

$$\mathcal{L}\{K_I(t)\} = \frac{\mathcal{L}\{\rho(t)\phi(t)\}}{\mathcal{L}\{\phi(t)\}} = \frac{\tau^{-\beta}s^{1-\beta}\mathcal{L}\{\phi(t)\}}{\mathcal{L}\{\phi(t)\}} = s^{1-\beta}\tau^{-\beta}. \tag{5.34}$$

Using the relation between the Riemann-Liouville fractional derivative and it's Laplace transform, Eq. (2.59), we are able to express the first integral of Eq. (5.25) as,

$$\int_0^t K_I(t-t')\frac{I(t')}{\theta(t',0)}dt' = \tau^{-\beta}\,{}_0\mathcal{D}_t^{1-\beta}\left(\frac{I(t)}{\theta(t,0)}\right). \tag{5.35}$$

Substituting Eqs. (5.35) and (5.30) into the master equations Eqs. (5.24), (5.25) and (5.26) yields the fractional-order infectivity and recovery SIR model,

$$\frac{dS(t)}{dt} = \lambda(t) - \frac{\omega(t)S(t)\theta(t,0)}{\tau^{\beta}}\,{}_0\mathcal{D}_t^{1-\beta}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma(t)S(t), \tag{5.36}$$

$$\frac{dI(t)}{dt} = \frac{\omega(t)S(t)\theta(t,0)}{\tau^{\beta}}\,{}_0\mathcal{D}_t^{1-\beta}\left(\frac{I(t)}{\theta(t,0)}\right) - \frac{\theta(t,0)}{\tau^{\alpha}}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma(t)I(t), \tag{5.37}$$

$$\frac{dR(t)}{dt} = \frac{\theta(t,0)}{\tau^{\alpha}}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma(t)R(t). \tag{5.38}$$

5.4 Reduction to Classic and Fractional Recovery SIR Models

Both the classic SIR and fractional recovery model are special cases of our derived Eqs. (5.36), (5.37) and (5.38). In this Section we consider the parameters required for the classic and fractional recovery SIR and how they relate to the generalised fractional model we have derived above. The classic SIR model can be obtained by taking constant functions for the birth, death and time dependent infectivity rates, i.e. $\lambda(t) = \lambda$, $\gamma(t) = \gamma$ and $\omega(t) = \omega$, respectively and taking the limit as $\alpha, \beta \to 1$. Noting that the limit,

$$\lim_{\alpha\to 1}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right) = \frac{I(t)}{\theta(t,0)}, \tag{5.39}$$

we obtain the classic SIR equations,

$$\frac{dS(t)}{dt} = \lambda - \frac{\omega}{\tau} S(t)I(t) - \gamma S(t), \tag{5.40}$$

$$\frac{dI(t)}{dt} = \frac{\omega}{\tau} S(t)I(t) - \frac{1}{\tau} I(t) - \gamma I(t), \tag{5.41}$$

$$\frac{dR(t)}{dt} = \frac{1}{\tau} I(t) - \gamma R(t). \tag{5.42}$$

By considering the relationship between the fractional exponents α and β and Eqs. (5.28) and (5.33), we gain insight into the underlying stochastic process of the classic SIR model. For $\alpha = 1$, the waiting time function, Eq. (5.28) reduces to an exponential function,

$$\phi(t) = e^{-\frac{t}{\tau}}. \tag{5.43}$$

Taking the limit $\beta \to 1$ the age of infection dependent infectivity, Eq. (5.33) becomes a constant,

$$\rho(t) = \lim_{\beta \to 1} \frac{\tau^{-\beta}}{\phi(t)} {}_0\mathcal{D}_t^{1-\beta} \phi(t) = \frac{1}{\tau}. \tag{5.44}$$

Note that this limit is independent of the form of $\phi(t)$.

In a similar fashion we obtain the fractional recovery SIR model [21] by taking the limit $\beta \to 1$, whilst leaving $0 < \alpha \leq 1$. Making use of the limit in Eq. (5.39) and the functional form of $\rho(t)$ from Eq. (5.44), we obtain,

$$\frac{dS(t)}{dt} = \lambda(t) - \frac{\omega}{\tau} S(t)I(t) - \gamma(t)S(t), \tag{5.45}$$

$$\frac{dI(t)}{dt} = \frac{\omega}{\tau} S(t)I(t) - \frac{\theta(t,0)}{\tau^\alpha} {}_0\mathcal{D}_t^{1-\alpha} \left(\frac{I(t)}{\theta(t,0)} \right) - \gamma(t)I(t), \tag{5.46}$$

$$\frac{dR(t)}{dt} = \frac{\theta(t,0)}{\tau^\alpha} {}_0\mathcal{D}_t^{1-\alpha} \left(\frac{I(t)}{\theta(t,0)} \right) - \gamma(t)R(t). \tag{5.47}$$

While the fractional recovery SIR model can be obtained from the general fractional infectivity and fractional recovery SIR model, we are unable to obtain the fractional infectivity SIR model [20]. The fractional infectivity SIR model requires $\alpha = 1$ and $0 < \beta < 1$, hence $\beta < \alpha$ violating our non-negativity conditions for $\rho(t)$.

A different form of $\rho(t)$ was considered in [20]. The form of the fractional infectivity in [20] could not readily be generalized to include a fractional recovery. Thus the model here with both fractional recovery with fractional infectivity provides an alternate form of fractional infectivity. The choice of which type of fractional infectivity model should be used could only be decided by comparisons with data.

5.5 Equilibrium State Analysis

The set of fractional-order infectivity and recovery SIR Eqs. (5.36), (5.37) and (5.38) are a non-autonomous dynamical system due to both the history dependence of the fractional derivative and the time dependence of the parameters. To find the equilibrium states we will simplify the model by taking all time dependent parameters to be constants, i.e. $\lambda(t) = \lambda$, $\gamma(t) = \gamma$ and $\omega(t) = \omega$. Hence the simplified master equations become,

$$\frac{dS(t)}{dt} = \lambda - \frac{\omega S(t)\theta(t,0)}{\tau^{\beta}}\,{}_0\mathcal{D}_t^{1-\beta}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma S(t), \tag{5.48}$$

$$\frac{dI(t)}{dt} = \frac{\omega S(t)\theta(t,0)}{\tau^{\beta}}\,{}_0\mathcal{D}_t^{1-\beta}\left(\frac{I(t)}{\theta(t,0)}\right) - \frac{\theta(t,0)}{\tau^{\alpha}}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma I(t), \tag{5.49}$$

$$\frac{dR(t)}{dt} = \frac{\theta(t,0)}{\tau^{\alpha}}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\frac{I(t)}{\theta(t,0)}\right) - \gamma R(t). \tag{5.50}$$

The constant recovery rate allows us to write Eq. (5.6) as,

$$\theta(t,0) = e^{-\gamma t}. \tag{5.51}$$

For an equilibrium state, (S^*, I^*, R^*), to exist the following limits must exist,

$$\lim_{t\to\infty} S(t) = S^*, \qquad \lim_{t\to\infty} I(t) = I^*, \qquad \lim_{t\to\infty} R(t) = R^*. \tag{5.52}$$

Taking the limit as $t \to \infty$ Eqs. (5.48), (5.49) and (5.50), reduce to,

$$0 = \lambda - \lim_{t\to\infty} \omega\tau^{-\beta} S(t) e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\beta}\left(e^{\gamma t} I(t)\right) - \gamma S^*, \tag{5.53}$$

$$0 = \lim_{t\to\infty} \omega\tau^{-\beta} S(t) e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\beta}\left(e^{\gamma t} I(t)\right) - \lim_{t\to\infty} e^{-\gamma t}\tau^{-\alpha}\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t} I(t)\right) - \gamma I^*, \tag{5.54}$$

$$0 = \lim_{t\to\infty} e^{-\gamma t}\tau^{-\alpha}\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t} I(t)\right) - \gamma R^*. \tag{5.55}$$

We use the result of [21] to evaluate the limit,

$$\lim_{t\to\infty} e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\alpha}\left(e^{\gamma t} I(t)\right) = \gamma^{1-\alpha} I^*. \tag{5.56}$$

The remaining limit can be split into,

$$\lim_{t\to\infty} S(t) e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\beta}\left(e^{\gamma t} I(t)\right) = \left(\lim_{t\to\infty} S(t)\right)\left(\lim_{t\to\infty} e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\beta}\left(e^{\gamma t} I(t)\right)\right). \tag{5.57}$$

Trivially we have $\lim_{t\to\infty} S(t) = S^*$, hence,

$$\lim_{t\to\infty} S(t) e^{-\gamma t}\, {}_0\mathcal{D}_t^{1-\beta}\left(e^{\gamma t} I(t)\right) = \gamma^{1-\beta} S^* I^*. \tag{5.58}$$

Substituting Eq. (5.58) into Eqs. (5.53), (5.54) and (5.55) yields,

$$0 = \lambda - \omega\tau^{-\beta}\gamma^{1-\beta} S^* I^* - \gamma S^*, \tag{5.59}$$

$$0 = \omega\tau^{-\beta}\gamma^{1-\beta} S^* I^* - \tau^{-\alpha}\gamma^{1-\alpha} I^* - \gamma I^*, \tag{5.60}$$

$$0 = \tau^{-\alpha}\gamma^{1-\alpha} I^* - \gamma R^*. \tag{5.61}$$

These equations permit two distinct equilibrium states, a disease free state,

$$S^* = \frac{\lambda}{\gamma}, \quad I^* = 0, \quad R^* = 0, \tag{5.62}$$

and an endemic state,

$$S^* = \frac{(\tau\gamma)^{-\alpha}+1}{\omega(\tau\gamma)^{-\beta}}, \quad I^* = \frac{\lambda}{\gamma\left((\tau\gamma)^{-\alpha}+1\right)} - \frac{1}{\omega(\tau\gamma)^{-\beta}},$$
$$R^* = (\tau\gamma)^{-\alpha}\left(\frac{\lambda}{\gamma\left((\tau\gamma)^{-\alpha}+1\right)} - \frac{1}{\omega(\tau\gamma)^{-\beta}}\right). \tag{5.63}$$

For all valid values of the parameters the disease free state will give non-negative populations and hence be physically obtainable. The same is not true of the endemic state, which is only physically obtainable if,

$$\frac{\lambda\omega}{(\tau\gamma)^{-\alpha}+1} > \tau^{\beta}\gamma^{\beta+1}. \tag{5.64}$$

In the case where $\alpha = \beta = 1$ the equilibrium states recover the equilibrium states of the standard SIR ODE model with vital dynamics. We expect that the endemic state will be asymptotically stable when it is physically obtainable in a similar manner to the endemic state for the fractional recovery SIR model [21].

5.5.1 Basic Reproduction Number

It is also possible to calculate the basic reproduction number for this model. This is defined as the expected number of individuals who will become infected from a single infectious individual in an otherwise uninfected population. This can be calculated from,

$$R_0 = \int_0^{\infty} \frac{\omega N\theta(t,0)}{\tau^{\beta}}\, {}_0\mathcal{D}_t^{1-\beta}\left(\frac{I_0(t)}{\theta(t,0)}\right), \tag{5.65}$$

where N is the total equilibrium population. From Eq. (5.9), with $i(-t,0) = \delta(-t)$, we have,

$$I_0(t) = e^{-\gamma t}E_{\alpha,1}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right). \tag{5.66}$$

It is then left to solve,

$$R_0 = \int_0^{\infty} \frac{\omega N e^{-\gamma t}}{\tau^{\beta}}\, {}_0\mathcal{D}_t^{1-\beta}\left(E_{\alpha,1}\left(-\left(\frac{t}{\tau}\right)^{\alpha}\right)\right). \tag{5.67}$$

The fractional derivative of the Mittag-Leffler function is well known and hence this can be simplified to,

$$R_0 = \int_0^\infty \frac{\omega N e^{-\gamma t}}{\tau^\beta} t^{\beta-1} E_{\alpha,\beta}\left(-\left(\frac{t}{\tau}\right)^\alpha\right). \tag{5.68}$$

This integral is now in a standard form and has solution [58],

$$R_0 = \frac{\omega N}{\tau^\beta}\left(\frac{\gamma^{\alpha-\beta}}{\gamma^\alpha + \tau^{-\alpha}}\right). \tag{5.69}$$

We can also rewrite the existence criterion for the endemic steady state, Eq. (5.64), in terms of R_0 by noting that the equilibrium population is $N = \frac{\lambda}{\gamma}$, giving,

$$R_0 > 1. \tag{5.70}$$

5.6 Summary

In this Chapter we have derived a fractional infectivity and recovery model using a stochastic process. The fractional derivatives arise as a consequence of taking an age-of-infection dependent infectivity and recovery to be power-law distributed. In doing so we have shown how to incorporate fractional derivatives into the model without violating the physicality of the parameters of the model. Under appropriate limits we are able to simplify this generalised fractional model to the fractional recovery and classic SIR models, however the fractional infectivity SIR model can't be recovered. We have shown the conditions under which an endemic steady state exists. The model and it's parameters are well posed and physical, however the fractional derivatives originated from power-law assumptions, and these assumptions need to be tested by fitting to data.

Chapter 6

Discretisation of the Fractional Recovery SIR Model

6.1 Introduction

This Chapter follows the discretisation of the fractional recovery SIR published in [21]. Starting with a discrete time stochastic process formulation of the fractional recovery SIR model we derive a numerical method for solving the governing fractional order differential equations. The numerical method is related to the discrete time stochastic process method that was introduced to solve the fractional Fokker-Planck equation [12]. We have implemented the numerical scheme to investigate the effects of changes in the fractional-order exponent on the qualitative behaviour of solutions. The numerical solutions converge to the calculated equilibrium states of the fractional recovery SIR model, when the parameters are constants. In Section 6.2 a stable numerical scheme for solving the fractional recovery SIR model is derived from a discrete time formulation of the stochastic process. Numerical solutions are investigated in Section 6.3 and in Section 6.4 the discrete time formulation is shown to converge, under a continuous time limit, to the continuous time formulation of Chapter 2.

6.2 SIR as a Discrete Time Random Walk

There are numerous numerical methods that have been developed for solving fractional-order differential equations [115, 121, 41] and many of these methods could be adapted to the system under consideration here. However recently we

showed that in the case where the fractional-order derivatives have been derived from CTRWs it is useful to reformulate the problem using DTRWs and then use this formulation as the basis of a numerical method [13]. The advantage of basing the numerical method on a discrete time stochastic process is that the derived explicit numerical method is easy to implement and is also inherently stable.

6.2.1 Discrete Time Random Walk

We consider a discrete time random walk where the walking particle is an individual that will transition though the S, I, and R, compartments. In order to obtain a useful numerical scheme from this we need the discrete time process to limit to the continuum process as the time step, Δt, goes to zero. This necessitates a slight modification to the transitions that were considered in the continuum case. Individuals are born into the susceptible compartment with a birth rate $\lambda(t)$ so that the number of individuals being born on the n^{th} time step, between time t and $t+\Delta t$, is equal to $\Lambda(n) = \lambda(t)\Delta t$. The probability that an individual will die and be removed from consideration on the n^{th} time step is $\gamma(n)$. Susceptible individuals who come in contact with an infected individual may become infected. The probability of an infected individual coming in contact and infecting a susceptible individual in the n^{th} time step is $\omega(n)$.

The recovery of infected individuals is assumed to be dependent on the number of time steps since they entered the infectious compartment. The individual is assumed to wait in the infectious compartment with a probability of "jumping" that is dependent on the time step. When a transition event occurs there are two possible things that can happen to the individual, they will either move to the recovered compartment or re-enter the infectious compartment with the transition probability, dependent on the time step, being reset. If the individual was infected before the first time step they will always transition to the recovered compartment. This self jump modification is required to ensure appropriate scaling as the size of the time step tends to zero. The probability of transitioning to the R compartment,

given a jump occurred, is denoted by r. The probability of jumping on the n^{th} step, conditional on not having jumped in the first $(n-1)$ steps, is denoted by $\mu(n)$.

From this it follows that the probability flux entering the I compartment on the n^{th} time step can be written as

$$\begin{aligned} Q_I^+(n) = &\sum_{k=-\infty}^{n-1} \omega(n)S(n-1)\phi(n-1-k)\theta(n-1,k)Q_I^+(k) \\ &+ (1-r)\sum_{k=1}^{n-1} \mu(n-k)\phi(n-1-k)\theta(n,k)Q_I^+(k). \end{aligned} \tag{6.1}$$

In the above equation, $\phi(n-k)$ is the probability of not jumping for $(n-k)$ steps and $\theta(n,k)$ is the probability that an individual who entered the I compartment on the k^{th} step has survived the death process up to the n^{th} step. If we assume that we have an initial distribution of infectious individuals at the 0^{th} time step, then we can infer that the flux at earlier times is given by,

$$Q_I^+(n) = \frac{i(-n,0)}{\theta(0,-n)\phi(-n)} \quad \forall n \leq 0. \tag{6.2}$$

Here $i(n,0)$ is the number of individuals at time step 0 who have been infected since time step n, with $n \leq 0$. This allows us to write the flux for $n > 0$ as

$$\begin{aligned} Q_I^+(n) = &\omega(n)S(n-1)\sum_{k=1}^{n-1} \phi(n-1-k)\theta(n-1,k)Q_I^+(k) \\ &+ (1-r)\sum_{k=1}^{n-1} \mu(n-k)\phi(n-1-k)\theta(n,k)Q_I^+(k) \\ &+ \omega(n)S(n-1)\theta(n-1,0)\sum_{k=-\infty}^{0} \phi(n-1-k)\frac{i(-k,0)}{\phi(-k)}. \end{aligned} \tag{6.3}$$

We can easily see that

$$\phi(n-k) = \prod_{j=0}^{n-k}(1-\mu(j)), \tag{6.4}$$

and

$$\theta(n,k) = \prod_{j=k}^{n}(1-\gamma(j)). \tag{6.5}$$

The number of individuals in the I compartment on the n^{th} time step is

$$I(n) = \sum_{k=1}^{n} \phi(n-k)\theta(n,k)Q_I^+(k) + I_0(n). \tag{6.6}$$

where,

$$I_0(n) = \theta(n,0) \sum_{k=-\infty}^{0} \phi(n-k)\frac{i(-k,0)}{\phi(-k)}. \tag{6.7}$$

Subtracting $I(n-1)$ from each side of Eq. (6.6) gives,

$$\begin{aligned} I(n) - I(n-1) =& Q_I^+(n) + \sum_{k=1}^{n-1}(\phi(n-k)\theta(n,k) - \phi(n-1-k)\theta(n-1,k))Q_I^+(k) \\ &+ I_0(n) - I_0(n-1), \end{aligned} \tag{6.8}$$

and substituting Eq. (6.3) into the right hand side of Eq. (6.8) and using Eq.(6.6) gives,

$$\begin{aligned} I(n) - I(n-1) =& \omega(n)S(n-1)I(n-1)) + I_0(n) - I_0(n-1) \\ &+ (1-r)\sum_{k=1}^{n-1}\mu(n-k)\phi(n-1-k)\theta(n,k)Q_I^+(k) \\ &+ \sum_{k=1}^{n-1}(\phi(n-k)\theta(n,k) - \phi(n-1-k)\theta(n-1,k))Q_I^+(k) \end{aligned} \tag{6.9}$$

Noting that,

$$\begin{aligned} \phi(n-k)\theta(n,k) - \phi(n-1-k)\theta(n-1,k) =& -\gamma(n)\phi(n-1-k)\theta(n-1,k) \\ &- \mu(n-k)\phi(n-1-k)\theta(n,k). \end{aligned} \tag{6.10}$$

we get,

$$\begin{aligned} I(n) - I(n-1) =& \omega(n)S(n-1)I(n-1) - \gamma(n)(I(n-1) - I_0(n-1)) \\ &+ I_0(n) - I_0(n-1) - r\sum_{k=1}^{n-1} \mu(n-k)\phi(n-1-k)\theta(n,k)Q_I^+(k). \end{aligned} \tag{6.11}$$

To simplify further we mirror the derivation in the CTRW approach, using the semi-group property of the death survival function, and using discrete Z-transform methods to replace the memory kernels. The Z-transform form n to z of $Y(n)$ is defined by [71],

$$\mathcal{Z}[Y(n)|z] = \sum_{n=0}^{\infty} Y(n)z^{-n}. \tag{6.12}$$

First we use the result

$$\theta(n,0) = \theta(n,k)\theta(k,0), \tag{6.13}$$

in Eq. (6.11) to write

$$\begin{aligned} I(n) - I(n-1) =& \omega(n)S(n-1)I(n-1) + I_0(n) - I_0(n-1) \\ &- \gamma(n)(I(n-1) - I_0(n-1)) - r\theta(n,0)\sum_{k=1}^{n-1} \mu(n-k)\phi(n-1-k)\frac{Q_I^+(k)}{\theta(k,0)}. \end{aligned} \tag{6.14}$$

and we use the same result in Eq. (6.6) to write

$$\frac{I(n) - I_0(n)}{\theta(n,0)} = \sum_{k=1}^{n} \phi(n-k)\frac{Q_I^+(k)}{\theta(k,0)}. \tag{6.15}$$

Finally, we need to express the sum $\sum_{k=1}^{n-1} \mu(n-k)\phi(n-1-k)\frac{Q_I^+(k)}{\theta(k,0)}$, in terms of $I(n)$ so we take the Z-transform of Eq. (6.15), and use the convolution property of Z-transforms to give,

$$\mathcal{Z}\left[\frac{I(n) - I_0(n)}{\theta(n,0)}|z\right] = \mathcal{Z}\left[\phi(n)|\, z\right]\mathcal{Z}\left[\frac{Q_I^+(n)}{\theta(n,0)}|z\right]. \tag{6.16}$$

We can now write

$$\sum_{k=0}^{n-1}\mu(n-k)\phi(n-1-k)\frac{Q_I^+(k)}{\theta(k,0)}=\sum_{k=0}^{n-1}\kappa(n-1-k)\frac{I(k)-I_0(k)}{\theta(k,0)}, \tag{6.17}$$

where,

$$\kappa(n)=\mathcal{Z}^{-1}\left[\frac{\mathcal{Z}\left[\mu(n)\phi(n-1)|z\right]}{\mathcal{Z}\left[\phi(n)|z\right]}\middle|n\right]. \tag{6.18}$$

The discrete time generalised master equation for an arbitrary waiting time distribution can then finally be found by substituting Eq. (6.17) into Eq. (6.14) to give,

$$\begin{aligned}I(n)-I(n-1)=&\omega(n)S(n-1)I(n-1)-\gamma(n)(I(n-1)-I_0(n-1))\\&+I_0(n)-I_0(n-1)-r\theta(n,0)\sum_{k=1}^{n-1}\kappa(n-k)\frac{I(k)-I_0(k)}{\theta(k,0)}.\end{aligned} \tag{6.19}$$

The master equations for the other compartments can be found by again considering a flux balance so that,

$$S(n)-S(n-1)=\Lambda(n)-\omega(n)S(n-1)I(n-1)-\gamma(n)S(n-1), \tag{6.20}$$

$$\begin{aligned}R(n)-R(n-1)=&r\theta(n,0)\sum_{k=1}^{n-1}\kappa(n-k)\frac{I(k)-I_0(k)}{\theta(k,0)}\\&+I_0(n)-I_0(n-1)+\gamma(n)I_0(n-1)-\gamma(n)R(n-1).\end{aligned} \tag{6.21}$$

6.2.2 Discrete Time Fractional Recovery SIR Model

The continuous time fractional recovery SIR model was obtained by considering Mittag-Leffler waiting time densities in the CTRW formulation. In the DTRW formulation a discrete time fractional recovery SIR model is obtained by considering a Sibuya(α) waiting time distribution [139, 13]. In this case the probability of jumping on the n^{th} time step, conditional on not having jumped on the previous

$n-1$ time steps, is given by

$$\mu(n) = \begin{cases} 0, & n = 0, \\ \frac{\alpha}{n}, & n > 0, \end{cases} \tag{6.22}$$

and the jump survival probability is given by

$$\phi(n) = \frac{\Gamma(1-\alpha+n)}{\Gamma(n+1)\Gamma(1-\alpha)}. \tag{6.23}$$

It is a simple matter to obtain the Z-transforms from n to z

$$\mathcal{Z}\left[\phi(n)|z\right] = \left(\frac{z-1}{z}\right)^{\alpha-1} \tag{6.24}$$

and

$$\begin{aligned} \mathcal{Z}\left[\mu(n)\phi(n-1)|z\right] &= \sum_{n=0}^{\infty} \mu(n)\phi(n-1)z^{-n} \\ &= \sum_{n=1}^{\infty} \mu(n)\phi(n-1)z^{-n} \\ &= 1 - \left(\frac{z-1}{z}\right)^{\alpha}. \end{aligned} \tag{6.25}$$

Now using Eq. (6.18) we have

$$\kappa(n) = \mathcal{Z}^{-1}\left[(1-z^{-1})^{1-\alpha} - (1-z^{-1})|n\right] \tag{6.26}$$

and then after taking the inverse Z-transform we obtain the fractional memory kernel

$$\kappa(n) = \delta_{1,n} + \frac{\Gamma(n-1+\alpha)}{\Gamma(\alpha-1)\Gamma(n+1)}. \tag{6.27}$$

This memory kernel can be calculated recursively by noting that for $n \geq 3$,

$$\kappa(n) = \left(1 + \frac{\alpha-2}{n}\right)\kappa(n-1). \tag{6.28}$$

The first two values are simply $\kappa(2) = \frac{\alpha}{2}(\alpha - 1)$and $\kappa(1) = \alpha$.

The number of initially infected individuals left at the n^{th} time step, $I_0(n)$, is found from Eq. (6.7) for the case $0 < \alpha < 1$,

$$I_0(n) = \theta(n, 0) \sum_{k=-\infty}^{0} \frac{\Gamma(1-k)\Gamma(1-k+n-\alpha)}{\Gamma(1-k+n)\Gamma(1-k-\alpha)} i(-k, 0). \tag{6.29}$$

In the case where the initially infected individuals were all infected at time zero this will simplify. Taking $i(-k, 0) = i_0\delta_{k,0}$ where i_0 is a constant and $\delta_{k,0}$ is a Kronecker Delta function, we find,

$$I_0(n) = \theta(n, 0) \frac{\Gamma(1+n-\alpha)}{\Gamma(1+n)\Gamma(1-\alpha)} i_0. \tag{6.30}$$

Again this may be also expressed recursively,

$$I_0(n) = \left(1 - \frac{\alpha}{n}\right) I_0(n-1), \tag{6.31}$$

with the initial condition, $I_0(0) = i_0$.

When $\alpha = 1$, $\phi(n) = 0$, for all $n > 0$, as such care has to be taken with the definition of $I_0(n)$. In this case the only physically permitted initial condition is that the initially infected individuals were all infected at time zero. Hence, when $\alpha = 1$, $I_0(n) = 0$ for $n > 0$, and $I_0(0) = i_0$.

The discrete time fractional recovery SIR model is obtained by using the memory kernel, Eq. (6.27), in Eqs. (6.19), (6.20), and (6.21).

In Appendix B we show that the discrete time fractional recovery SIR model equations limit to the fractional recovery SIR model equations by identifying $t = n\Delta t$ and taking the limit $\Delta t \to 0$ and $r \to 0$, with

$$\lim_{\Delta t, r \to 0} \frac{r}{\Delta t^{\alpha}} = \mu. \tag{6.32}$$

This justifies our use of the explicit discrete time model equations as a numerical method for solving the continuous time fractional recovery SIR model.

6.2.3 Equivalence Between The Discrete and Continuous Parameters

As the discrete fractional recovery SIR governing equations, Eqs. (6.20), (6.19), and (6.21) with Eq. (6.27), limit to the continuous time fractional recovery SIR model equations we can approximate the solution of the continuous time equations with the solution to the discrete time equations. Given a set of parameters for the continuous time equations we need to identify corresponding values of the parameters in the discrete time equations. The continuous time fractional recovery SIR model is parameterised by three functions, ($\lambda(t)$, $\omega(t)$, $\gamma(t)$), and two constants (α, μ). The discrete time fractional recovery SIR model is parameterised by three functions ($\Lambda(n)$, $\omega(n)$, $\gamma(n)$), and three constants (α, r, Δt). Assuming a given time step Δt, the correspondence between the continuous time t and the discrete time n is given by $t = n\Delta t$. The expected number of births in a time step is related to the continuous time birth rate by,

$$\Lambda(n) = \Delta t \lambda(n\delta t). \tag{6.33}$$

The probability of an individual becoming infected in a time step is related to the continuous time infection rate by,

$$\omega(n) = 1 - \exp\left(- \int_{n\delta t}^{(n+1)\Delta t} \omega(t')\, dt' \right). \tag{6.34}$$

We can treat the death probability in a similar fashion,

$$\gamma(n) = 1 - \exp\left(- \int_{n\delta t}^{(n+1)\Delta t} \gamma(t')\, dt' \right). \tag{6.35}$$

This definition of the death probability ensures that the discrete survival function, $\theta(n, m)$ is equal to the continuous time survival function evaluated at $n\delta t$ $m\delta t$, i.e.

$$\theta(n, m) = \exp\left(-\int_{m\Delta t}^{n\Delta t} \gamma(t')\, dt'\right). \tag{6.36}$$

The discrete anomalous exponent, α, is unchanged from the continuous case. The remaining parameter in the discrete model, r, is obtained from,

$$r = \mu \Delta t^{\alpha}, \tag{6.37}$$

which is consistent with Eq. (6.32). Note that r is a probability and as such is bound in the interval $[0, 1]$. Thus given the parameters μ and α from the continuous time model, Eq. (6.37) constrains Δt as follows,

$$\Delta t < \left(\frac{1}{\mu}\right)^{\frac{1}{\alpha}}. \tag{6.38}$$

Given that Eqs. (6.20), (6.19), and (6.21) are explicit difference equations if we know $S(k)$, $I(k)$, and $R(k)$, for $1 < k < n$, then we can calculate $S(n)$, $I(n)$, and $R(n)$. In this manner we have a simple numerical method that approximates the solution of the continuous time fractional recovery SIR model by simply noting that for $t = n\Delta t$, $S(t) \approx S(n)$, $I(t) \approx I(n)$, and $R(t) \approx R(n)$.

6.3 Example

We consider the fractional recovery SIR model, Eqs. (2.61), (2.62), and (2.63), with the following parameters, $\lambda(t) = 0.1$, $\omega(t) = 0.02$, $\gamma(t) = 0.001$, $\mu = 1$, and a range of $\alpha \in (0, 1]$. We also take a delta function initial condition at $t = 0$ for the infected population, $i(t, 0) = 0.5\delta(t)$. The initial recovered population is taken to be zero, $R(0) = 0$, and the initial population in the susceptible compartment is taken so that the total population is at the equilibrium level of 100, i.e. $S(0) = 99.5$. With these parameter values, the system has two possible steady states, the disease free steady

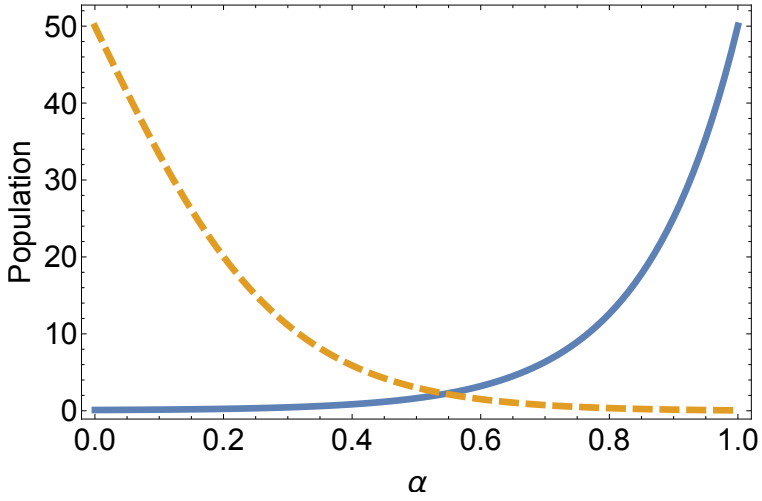

Figure 6.1: The endemic steady state in the fractional recovery SIR model plotted as a function of α for susceptibles (solid line) and infecteds (dashed line). The Parameters were $\lambda = 0.1$, $\omega = 0.02$, $\gamma = 0.001$.

state given by Eq. (2.84) and the endemic steady state given by Eq. (2.85). The endemic steady state for susceptibles and infecteds are plotted as a function of α in Fig. 6.1.

To find the numerical approximation for this situation we solve the discrete equations, Eqs. (6.20), (6.19), and (6.21). For a given Δt, the discrete parameters are taken to be $\Lambda(n) = 0.1\Delta t$, $\omega(n) = 1 - \exp(-0.02\Delta t)$, $\gamma(n) = 1 - \exp(-0.001\Delta t)$, and $r = \Delta t^{\alpha}$. The initial conditions are implemented by taking $S(0) = 99.5$, $R(0) = 0$, and $i(-k, 0) = 0.5\delta_{0,k}$.

In Fig. 6.2 we show plots of $S(t)$ and $I(t)$ versus time for $\alpha = 0.3, 0.5, 0.7, 0.9$ with initial conditions $S(0) = 99.5, I(0) = 0.5, R(0) = 0$. The number of susceptibles falls sharply over short times before rising slowly towards a steady state at later times. The number of infecteds rises to a maximum in the short time regime before declining slowly back towards a long time steady state. It can be seen that the peak level of infection and the long time levels of infection are both increased with decreasing α.

For values of α very close to one the numerical solutions show an oscillatory approach towards the steady state. This can be seen in Fig. 6.3 for $\alpha = 0.99$, 0.999,

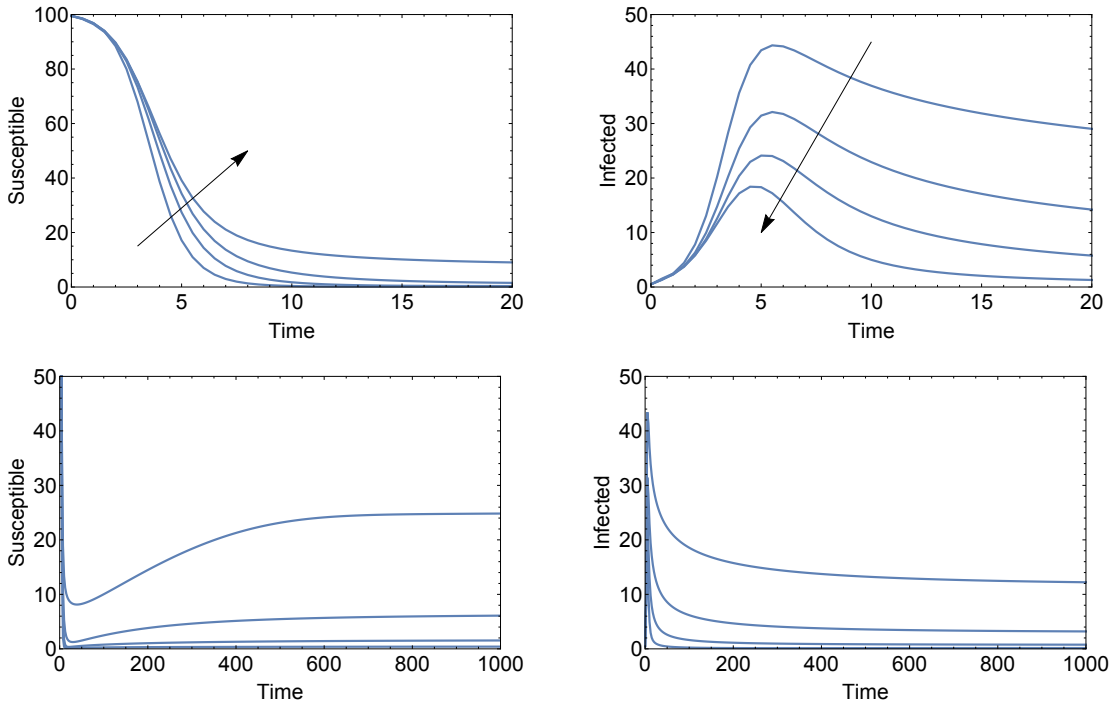

Figure 6.2: Plots of $S(t)$ and $I(t)$ versus time in the fractional recovery SIR model with $\alpha = 0.3, 0.5, 0.7, 0.9$. The arrow indicates the direction of increasing α. The other parameters are $\lambda = 0.1$, $\omega = 0.02$, $\gamma = 0.001$. The model was solved using the DTRW method with $\Delta t = 0.05$.

and 1. The oscillations are suppressed as α is decreased.

6.4 Limit To Continuous Time

The discrete time fractional recovery SIR model can be shown to limit to the fractional recovery SIR model by identifying $t = n\Delta t$ and taking the limit $\Delta t \to 0$ with $r/\Delta t^{\alpha}$ finite. The continuous time equations can be obtained from the discrete time equations using Z-star transform methods. The Z-star transform of $Y(n)$ is given by

$$Z^*[Y(n)|s, \Delta t] = \sum_{n=0}^{\infty} Y(n) e^{-ns\Delta t} \tag{6.39}$$

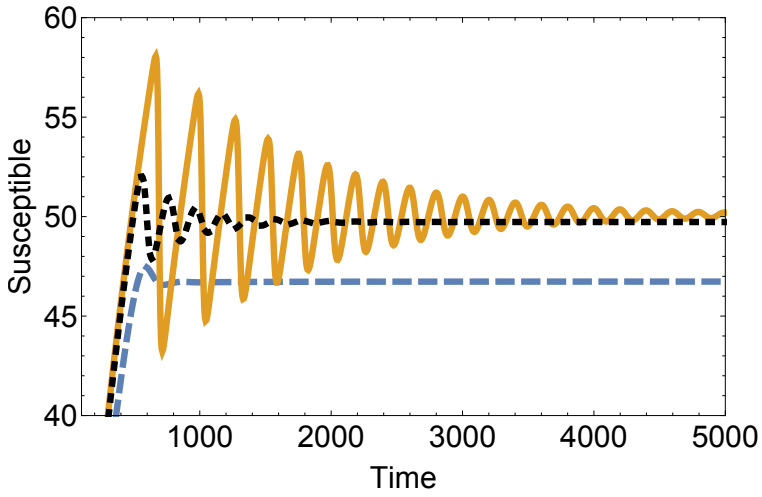

Figure 6.3: Plot of susceptible versus time, after the initial relaxation time, for $\alpha = 1$ (solid line), $\alpha = 0.999$ (dotted line) and $\alpha = 0.99$ (dashed line). The other parameters are $\lambda = 0.1$, $\omega = 0.02$, $\gamma = 0.001$, and $\Delta t = 0.05$.

It follows that

$$\begin{aligned} \Delta t Z^*[Y(n)|s,\Delta t] &= \sum_{n=0}^{\infty} Y(n) e^{-ns\Delta t}\Delta t \\ &= \sum_{n=0}^{\infty} \tilde{Y}(n\Delta t) e^{-ns\Delta t}\Delta t, \end{aligned} \tag{6.40}$$

where we have introduced $\tilde{Y}(t)$ as a function defined over a continuous variable t. We can now take the inverse Laplace transform from s to t

$$\mathcal{L}_s^{-1}\left[\Delta t Z^*[Y(n)|s,\Delta t]\middle| t\right] = \sum_{n=0}^{\infty} \tilde{Y}(n\Delta t)\delta(t-n\Delta t)\Delta t \tag{6.41}$$

where $\delta(t)$ is the Dirac delta function. Here, and in the following, we use the notation $\mathcal{L}_s^{-1}\left[Y(s)\middle| t\right]$ to denote the inverse Laplace transform from s to t and we use the notation $\mathcal{L}_t\left[Y(t)\middle| s\right]$ to denote the Laplace transform from t to s.

It is useful to define the function

$$\tilde{Y}(t|\Delta t) = \sum_{n=0}^{\infty} \tilde{Y}(n\Delta t)\delta(t-n\Delta t)\Delta t. \tag{6.42}$$

In a similar fashion we have

$$\begin{aligned}\mathcal{L}_s^{-1}\left[\Delta t Z^*[Y(n-1)|s,\Delta t]\middle|t\right] &= \sum_{n=0}^{\infty}\tilde{Y}(n\Delta t)\delta(t-(n+1)\Delta t)\Delta t \\ &= \sum_{n=0}^{\infty}\tilde{Y}((n-1)\Delta t)\delta(t-n\Delta t)\Delta t \\ &= \tilde{Y}(t-\Delta t|\Delta t).\end{aligned} \tag{6.43}$$

Note that, with $t' = n\Delta t$, in Eq. (6.42), we have

$$\begin{aligned}\lim_{\Delta t\to 0}\tilde{Y}(t|\Delta t) &= \lim_{\Delta t\to 0}\sum_{n=0}^{\infty}\tilde{Y}(n\Delta t)\delta(t-n\Delta t)\Delta t \\ &= \int_0^{\infty}\tilde{Y}(t')\delta(t-t')\,dt' \\ &= \tilde{Y}(t).\end{aligned} \tag{6.44}$$

This formally identifies

$$\tilde{Y}(t) = \lim_{\Delta t\to 0}\mathcal{L}_s^{-1}\left[\Delta t Z^*[Y(n)|s,\Delta t]\middle|t\right], \tag{6.45}$$

provided that the limit exists.

We further note the product rule

$$\begin{aligned}&\lim_{\Delta t\to 0}\sum_{n=0}^{\infty}\tilde{X}(n\Delta t)\tilde{Y}(n\Delta t)\delta(t-n\Delta t)\Delta t \\ &= \left(\lim_{\Delta t\to 0}\sum_{n=0}^{\infty}\tilde{X}(n\Delta t)\delta(t-n\Delta t)\Delta t\right)\left(\lim_{\Delta t\to 0}\sum_{n=0}^{\infty}\tilde{Y}(n\Delta t)\delta(t-n\Delta t)\Delta t\right),\end{aligned} \tag{6.46}$$

which equates to $\tilde{X}(t)\tilde{Y}(t)$ in each case, with $t' = n\Delta t$, provided that both $\tilde{X}(t)$ and $\tilde{Y}(t)$ exist.

We now take the inverse Laplace transform of the Z-star transform of Eq. (6.19) and multiply by $\frac{\Delta t}{\Delta t}$ to write

$$\begin{aligned}
&\sum_{n=0}^{\infty} \frac{\tilde{I}(n\Delta t) - \tilde{I}((n-1)\Delta t)}{\Delta t} \delta(t - n\Delta t)\Delta t \\
&= \sum_{n=0}^{\infty} \frac{\tilde{\omega}(n\Delta t)}{\Delta t} \tilde{S}((n-1)\Delta t)\tilde{I}((n-1)\Delta t)\delta(t - n\Delta t)\Delta t \\
&\quad - \frac{r}{\Delta t} \sum_{n=0}^{\infty} \tilde{\theta}(n\Delta t, 0) \left(\sum_{k=0}^{n-1} \tilde{\kappa}((n-k)\Delta t) \frac{\tilde{I}(k\Delta t) - \tilde{I}_0(k\delta t)}{\tilde{\theta}(k\Delta t, 0)} \right) \delta(t - n\Delta t)\Delta t \\
&\quad - \sum_{n=0}^{\infty} \frac{\tilde{\gamma}(n\Delta t)}{\Delta t} \left(\tilde{I}((n-1)\Delta t) - \tilde{I}_0((n-1)\delta t) \right) \delta(t - n\Delta t)\Delta t \\
&\quad + \sum_{n=0}^{\infty} \frac{\tilde{I}_0(n\Delta t) - \tilde{I}_0((n-1)\Delta t)}{\Delta t} \delta(t - n\Delta t)\Delta t.
\end{aligned} \tag{6.47}$$

We now take the continuous time limit of Eq. (6.47) using $t' = n\Delta t$ and the product rule in Eq. (6.46), to obtain

$$\begin{aligned}
&\int_0^{\infty} \left(\lim_{\Delta t \to 0} \frac{\tilde{I}(t') - \tilde{I}(t' - \Delta t)}{\Delta t} \right) \delta(t - t')\, dt' = \\
&\quad \int_0^{\infty} \hat{\omega}(t')\tilde{S}(t')\tilde{I}(t')\delta(t - t')\, dt' \\
&\quad - \left(\int_0^{\infty} \tilde{\theta}(t', 0)\delta(t - t')\, dt' \right) \left(\lim_{\Delta t \to 0} \frac{r}{\Delta t} \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n-1} \tilde{\kappa}((n-k)\Delta t) \frac{\tilde{I}(k\Delta t) - \tilde{I}_0(k\Delta t)}{\tilde{\theta}(k\Delta t, 0)} \right) \right. \\
&\quad \left. \times \delta(t - n\Delta t)\Delta t \right) - \int_0^{\infty} \hat{\gamma}(t') \left(\tilde{I}(t') - \tilde{I}_0(t') \right) \delta(t - t')\, dt' \\
&\quad + \int_0^{\infty} \left(\lim_{\Delta t \to 0} \frac{\tilde{I}_0(t') - \tilde{I}_0(t' - \Delta t)}{\Delta t} \right) \delta(t - t')\, dt'
\end{aligned} \tag{6.48}$$

where we have defined continuous time rate parameters

$$\hat{\omega}(t') = \lim_{\Delta t \to 0} \frac{\tilde{\omega}(n\Delta t)}{\Delta t}, \tag{6.49}$$

and

$$\hat{\gamma}(t') = \lim_{\Delta t \to 0} \frac{\tilde{\gamma}(n\Delta t)}{\Delta t}. \tag{6.50}$$

Equation (6.48) simplifies further to

$$\begin{aligned}\frac{d\tilde{I}(t)}{dt} &= \hat{\omega}(t)\tilde{S}(t)\tilde{I}(t) - \hat{\gamma}(t)\left(\tilde{I}(t) - \tilde{I}_0(t)\right) + \frac{d\tilde{I}_0(t)}{dt} \\ &\quad - \tilde{\theta}(t,0)\left(\lim_{\Delta t \to 0} \frac{r}{\Delta t} \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n-1} \tilde{\kappa}((n-k)\Delta t) \frac{\tilde{I}(k\Delta t) - \tilde{I}_0(k\Delta t)}{\tilde{\theta}(k\Delta t, 0)} \right) \delta(t - n\Delta t)\Delta t \right).\end{aligned} \tag{6.51}$$

The further reduction of this equation depends on the specific form of the memory kernel $\kappa(n)$. In the case of a jump at each time step the memory kernel is,

$$\kappa(n) = \delta_{n,1}. \tag{6.52}$$

In this case we can perform the sum over k explicitly in Eq. (6.51) to arrive at

$$\begin{aligned}\frac{d\tilde{I}(t)}{dt} &= \hat{\omega}(t)\tilde{S}(t)\tilde{I}(t) - \hat{\gamma}(t)\left(\tilde{I}(t) - \tilde{I}_0(t)\right) + \frac{d\tilde{I}_0(t)}{dt} \\ &\quad - \tilde{\theta}(t,0)\left(\lim_{\Delta t \to 0} \frac{r}{\Delta t} \sum_{n=0}^{\infty} \frac{\tilde{I}((n-1)\Delta t) - \tilde{I}_0((n-1)\Delta t)}{\tilde{\theta}((n-1)\Delta t, 0)} \delta(t - n\Delta t)\Delta t \right).\end{aligned} \tag{6.53}$$

In order for the continuous time limit of the above equation to exist we define

$$\mu = \lim_{\Delta t \to 0} \frac{r}{\Delta t}. \tag{6.54}$$

Note that r is a free parameter in the range $[0, 1]$ and hence μ is only well defined in this limit if we take r to be a function of Δt. With this definition of μ we can now perform the limit $\delta t \to 0$ to obtain the continuous time equation,

$$\frac{d\tilde{I}(t)}{dt} = \hat{\omega}(t)\tilde{S}(t)\tilde{I}(t) - \mu(\tilde{I}(t) - \tilde{I}_0(t)) - \hat{\gamma}(t)(\tilde{I}(t) - \tilde{I}_0(t)) + \frac{d\tilde{I}_0(t)}{dt}. \tag{6.55}$$

This further simplifies to

$$\frac{d\tilde{I}}{dt} = \hat{\omega}(t)\tilde{S}(t)\tilde{I}(t) - \mu\tilde{I}(t) - \hat{\gamma}(t)\tilde{I}(t). \tag{6.56}$$

Equation (6.56) recovers the corresponding equation in the classic SIR model.

We now consider the continuous time limit of Eq. (6.51) with the Sibuya memory kernel, given by Eq. (6.18). First we simplify the double sum in Eq. (6.51) using Laplace transforms and Z-transforms as follows:

$$\begin{aligned}
&\lim_{\Delta t\to 0} \frac{r}{\Delta t}\sum_{n=0}^{\infty}\left(\sum_{k=0}^{n-1}\tilde{\kappa}((n-k)\Delta t)\frac{\tilde{I}(k\Delta t)-\tilde{I}_0(k\Delta t)}{\tilde{\theta}(k\Delta t,0)}\right)\delta(t-n\Delta t)\Delta t \\
&= \mathcal{L}_s^{-1}\left[\mathcal{L}_t\left[\lim_{\Delta t\to 0} \frac{r}{\Delta t}\sum_{n=0}^{\infty}\left(\sum_{k=0}^{n-1}\tilde{\kappa}((n-k)\Delta t)\frac{\tilde{I}(k\Delta t)-\tilde{I}_0(k\Delta t)}{\tilde{\theta}(k\Delta t,0)}\right)\delta(t-n\Delta t)\Delta t\middle| s\right]\middle| t\right] \\
&= \mathcal{L}_s^{-1}\left[\lim_{\Delta t\to 0} \frac{r}{\Delta t}\sum_{n=0}^{\infty}\left(\sum_{k=0}^{n-1}\tilde{\kappa}((n-k)\Delta t)\frac{\tilde{I}(k\Delta t)-\tilde{I}_0(k\Delta t)}{\tilde{\theta}(k\Delta t,0)}\right)e^{-sn\Delta t}\Delta t\middle| t\right] \\
&= \mathcal{L}_s^{-1}\left[\lim_{\Delta t\to 0} \frac{r}{\Delta t}Z^*[\sum_{k=0}^{n-1}\kappa(n-k)\frac{I(k)-I_0(k)}{\theta(k,0)}|s,\Delta t]\Delta t\middle| t\right] \\
&= \mathcal{L}_s^{-1}\left[\lim_{\Delta t\to 0} \frac{r}{\Delta t}Z^*[\kappa(n)|s,\Delta t]Z^*[\frac{I(n)-I_0(k)}{\theta(n,0)}|s,\Delta t]\Delta t\middle| t\right].
\end{aligned} \tag{6.57}$$

The last line in the above follows from the convolution theorem for Z-star transforms.

To proceed further we use the Z-transform of the Sibuya memory kernel in Eq. (6.26) to write

$$\begin{aligned}
Z^*[\kappa(n)|s,\Delta t] &= \left[((1-e^{-s\Delta t})^{1-\alpha} - (1-e^{-s\Delta t}))\right] &(6.58)\\
&\approx (s\Delta t)^{1-\alpha} + o(s\Delta t). &(6.59)
\end{aligned}$$

The result in Eq. (6.57) can now be written as

$$\begin{aligned}
&\lim_{\Delta t\to 0}\frac{r}{\Delta t}\sum_{n=0}^{\infty}\left(\sum_{k=0}^{n-1}\tilde{\kappa}((n-k)\Delta t)\frac{\tilde{I}(k\Delta t)-\tilde{I}_0(k\Delta t)}{\tilde{\theta}(k\Delta t,0)}\right)\delta(t-n\Delta t)\Delta t\\
&=\mathcal{L}_s^{-1}\left[\lim_{\Delta t\to 0}\frac{r}{\Delta t^{\alpha}}s^{1-\alpha}\sum_{n=0}^{\infty}\frac{\tilde{I}(n\Delta t)-\tilde{I}_0(n\Delta t)}{\tilde{\theta}(n\Delta t,0)}e^{-sn\Delta t}\Delta t\middle| t\right]\\
&=\mu\mathcal{L}_s^{-1}\left[s^{1-\alpha}\int_0^{\infty}\frac{\tilde{I}(t)-\tilde{I}_0(t)}{\tilde{\theta}(t,0)}e^{-st}\,dt\middle| t\right]\\
&=\mu\mathcal{L}_s^{-1}\left[s^{1-\alpha}\mathcal{L}_t\left[\frac{\tilde{I}(t)-\tilde{I}_0(t)}{\tilde{\theta}(t,0)}\middle| s\right]\middle| t\right],
\end{aligned}\tag{6.60}$$

where

$$\mu=\lim_{\Delta t\to 0}\frac{r}{\Delta t^{\alpha}}.\tag{6.61}$$

Finally we substitute the result of Eq. (6.60) into Eq. (6.51), and use the known result [121]

$$\mathcal{L}_t\left[{}_0D_t^{1-\alpha}Y(t)\middle| s\right]=s^{1-\alpha}\mathcal{L}_t\left[Y(t)\middle| s\right]\tag{6.62}$$

to invert the Laplace transform and obtain

$$\frac{d\tilde{I}(t)}{dt}=\hat{\tilde{\omega}}(t)\tilde{S}(t)\tilde{I}(t)-\mu\hat{\tilde{\theta}}(t,0)\,{}_0D_t^{1-\alpha}\left(\frac{\tilde{I}(t)-\tilde{I}_0(t)}{\hat{\tilde{\theta}}(t,0)}\right)-\hat{\tilde{\gamma}}(t)\left(\tilde{I}(t)-\tilde{I}_0(t)\right)+\frac{d\tilde{I}_0(t)}{dt}.\tag{6.63}$$

Equation (6.63) recovers the continuous time fractional recovery SIR model equation.

Note that in order for the continuous time limit of the fractional recovery SIR model equation to exist we defined,

$$\mu=\lim_{\Delta t\to 0}\frac{r}{\Delta t^{\alpha}},\tag{6.64}$$

which requires $r\in[0,1]$ to be a function of Δt. This is important for numerical simulations based on this DTRW method where we take $r=\mu\Delta t^{\alpha}$ and then the requirement that $r\in[0,1]$ places restrictions on Δt for given α and μ.

6.5 Summary

We have derived a discrete time fractional recovery model that limits to the continuous time fractional-order model as the time step goes to zero. The discrete time model was itself derived from a stochastic process and we have used this model to provide a stable numerical solver for the continuous time model. Our numerical solutions based on this discrete model show that the prevalence of infection and the peak levels of infection are both elevated by the fractional-order derivative as it is varied further away from the integer order derivative in the classic SIR model.

Chapter 7

Discretisation of the Fractional General Compartment Model

7.1 Introduction

The work in this Chapter follows the publication [19]. We have introduced an approach for finding solutions of fractional order compartment models that also provides further insight into stochastic modelling. Our approach is based on using the correspondence between continuous time, and discrete time, stochastic processes. The fractional order compartment models of the type derived form a continuous time stochastic process in Chapter 3 can also be derived from a corresponding discrete time stochastic process. The discrete master equations, for the discrete time stochastic process can be used in turn to formulate stable numerical schemes that can easily be implemented to obtain approximate solutions for the continuous time fractional order compartment models. One of the purposes of this text is to draw attention to, and develop connections between, discrete time stochastic processes and numerical schemes.

The remainder of this Chapter is organized as follows. The governing evolution equation of a discrete time stochastic process for a single compartment is given in Section 7.2. A general compartment model can easily be formed from the composition of any number of single compartments. The only constraint that we place on the compartment models is that there is a single non-Markovian removal process for each compartment. This restriction is required in order to obtain fractional derivatives in the continuous time limit.

In Section 7.3 we show that the governing equations for the discrete time stochastic process will, in the limit of small time steps, approach the governing equation for a fractional order compartment model. This correspondence provides the basis for utilising the discrete time process as an approximation for the continuous time compartment model. In previous work [13, 9], the governing discrete time evolution equations were used directly to provide a difference equation approximation to the fractional order partial differential equations. This was possible as the particular choice of waiting time distributions led to an expression for the discrete time memory kernel that was amenable to simplification through Z-transforms. Here we consider choices of waiting time distributions where this simplification cannot be carried out. Instead, we track both the population in each compartment, as well as the flux between the compartments at each time step. By tracking the fluxes we obviate the need to perform the inverse Z-transformations required to calculate the memory kernel.

The single compartment model is extended to multiple compartments in Section 7.4, where we show that the multi compartment system can be considered via a flux matrix. The implementation of the numerical scheme for an arbitrary fractional order compartment model is given in Section 7.5. A general example is considered to illustrate how to construct both the fractional order compartment model PDE's as well as the numerical scheme for their solution.

In Section 7.6, particular examples are given to illustrate the use of the scheme. Examples are chosen for their tractability, so we can compare the method to exact solutions, and for their ability to demonstrate the variety of uses of compartment models.

7.2 Discrete Derivation

A general compartment model can be analyzed and solved by separating the structure into several single compartments [14]. As such we will develop our stochastic

process by considering the dynamics of a single compartment, before combining multiple single compartments into a full compartment model.

We begin by considering an ensemble of particles that enter the compartment, wait for a random number of time steps, drawn from a probability distribution, and then leave. In general the expected number of particles in the compartment after n time steps, $X(n)$, can be calculated as,

$$X(n) = \sum_{k=0}^{n} \Xi(n,k) Q(k), \tag{7.1}$$

where $Q(k)$ is the flux of entering particles on the k^{th} time step, and $\Xi(n,k)$ is the probability that a particle that entered the compartment on the k^{th} time step has survived until the n^{th} time step.

Considering the case where we have two independent processes that describe the waiting time, we may write the survival function, $\Xi(n,k)$ as the product of each processes survival functions,

$$\Xi(n,k) = \Theta(n,k)\Phi(n,k). \tag{7.2}$$

In order to obtain a fractional order compartment model we will take one of our processes to be Markovian, with survival function $\Theta(n,k)$, and the other to be non-Markovian with survival function $\Phi(n,k)$. The Markovian survival function will obey a semi-group property such that,

$$\Theta(n,k) = \Theta(n,m)\Theta(m,k), \tag{7.3}$$

with integers $n > m > k$. The non-Markovian process is assumed to only depend on the amount of time that a particle has spent in the compartment, and as such we may write its survival function as,

$$\Phi(n,k) = \Phi(n-k) \tag{7.4}$$

The expected flux of particles in the compartment can be written as,

$$X(n)-X(n-1) = \sum_{k=0}^{n} \Theta(n,k)\Phi(n-k)Q(k) - \sum_{k=0}^{n-1} \Theta(n-1,k)\Phi(n-1-k)Q(k). \quad (7.5)$$

This in turn can be rewritten as,

$$\begin{aligned} X(n) - X(n-1) =& Q(n) - \sum_{k=0}^{n-1} \Phi(n-1-k)(\Theta(n-1,k) - \Theta(n,k))Q(k) \\ & - \sum_{k=0}^{n-1} \Theta(n,k)\Psi(n-k)Q(k), \end{aligned} \quad (7.6)$$

where the flux leaving the compartment has been split into a Markovin and a non-Markovain component, we have defined,

$$\Psi(n) = \Phi(n-1) - \Phi(n), \quad (7.7)$$

and used the fact that $\Theta(n,n) = 1$, and $\Phi(0) = 1$. Using the semi-group property, Eq. (7.3) this can be written,

$$\begin{aligned} X(n) - X(n-1) =& Q(n) - (1 - \Theta(n,n-1)) \sum_{k=0}^{n-1} \Theta(n-1,k)\Phi(n-1-k)Q(k) \\ & - \sum_{k=0}^{n-1} \Theta(n,k)\Psi(n-k)Q(k). \end{aligned} \quad (7.8)$$

It should be noted that the decomposition from Eq. (7.5) to Eq. (7.6) is not unique and the choice made is equivalent to requiring that a particle survive the Markovian process before it may leave due to the non-Markovian process. The alternate choice, or having the particle survive the non-Markovian process before leaving due to the Markovian process, could be made which would give a different form of Eq. (7.6). This choice should be considered as part of the definition of our overall stochastic process.

Equation (7.6) can be further simplified using Eq. (7.1) to give,

$$X(n)-X(n-1) = Q(n)-(1-\Theta(n,n-1))X(n-1)-\sum_{k=0}^{n-1}\Theta(n,k)\Psi(n-k)Q(k). \quad (7.9)$$

The last sum may be expressed as a convolution by noting the semi-group property of the Markov survival function, and taking $\Psi(0) = 0$, so that,

$$X(n) - X(n-1) = Q(n) - (1-\Theta(n,n-1))X(n-1) - \Theta(n,0)\sum_{k=0}^{n}\Psi(n-k)\frac{Q(k)}{\Theta(k,0)}. \quad (7.10)$$

We can further simplify this equation by considering the Z-transform of the discrete convolution on the right hand side. Firstly from Eqs. (7.1), (7.2) and (7.3) we have,

$$\frac{X(n)}{\Theta(n,0)} = \sum_{k=0}^{n}\Phi(n-k)\frac{Q(k)}{\Theta(k,0)}. \quad (7.11)$$

Taking the Z-transform of this equation then gives,

$$\mathcal{Z}\left\{\frac{X(n)}{\Theta(n,0)}\right\} = \mathcal{Z}\left\{\Phi(n)\right\}\mathcal{Z}\left\{\frac{Q(n)}{\Theta(n,0)}\right\}. \quad (7.12)$$

Taking the Z-transform of the convolution in Eq. (7.10) similarly gives,

$$\mathcal{Z}\left\{\sum_{k=0}^{n}\Psi(n-k)\frac{Q(k)}{\Theta(k,0)}\right\} = \mathcal{Z}\left\{\Psi(n)\right\}\mathcal{Z}\left\{\frac{Q(n)}{\Theta(n,0)}\right\}. \quad (7.13)$$

Combining these results we see that,

$$\sum_{k=0}^{n}\Psi(n-k)\frac{Q(k)}{\Theta(k,0)} = \sum_{k=0}^{n}K(n-k)\frac{X(k)}{\Theta(k,0)}, \quad (7.14)$$

where the memory kernel K is defined by its Z-transform,

$$\mathcal{Z}\left\{K(n)\right\} = \frac{\mathcal{Z}\left\{\Psi(n)\right\}}{\mathcal{Z}\left\{\Phi(n)\right\}}. \quad (7.15)$$

We can then write the master equation for the discrete time evolution of the probability as,

$$X(n)-X(n-1)=Q(n)-(1-\Theta(n,n-1))X(n-1)-\Theta(n,0)\sum_{k=0}^{n}K(n-k)\frac{X(k)}{\Theta(k,0)}. \tag{7.16}$$

7.3 Continuum Limits

The continuum limit of the discrete time master equation, Eq. (7.16), will be obtained by considering the limit as the time step size is decreased to zero. To begin we assume a form for the waiting time distribution by assuming that there exists a continuous time waiting time survival function, $\phi(t)$. Taking a lattice spacing Δt we define our discrete time waiting time survival function as,

$$\Phi(n)=\phi_{\Delta t}(n\Delta t)=\phi(n\Delta t), \tag{7.17}$$

where $\phi_{\Delta t}$ is a function over a continuous time such that at the points $t=n\Delta t$ it agrees with the discrete time function. Away from these points we will assume that the function is continuous via some form of interpolation. From the survival function we can find the discrete time probability mass function

$$\Psi(n)=\psi_{\Delta t}(n\Delta t)=\phi((n-1)\Delta t)-\phi(n\Delta t). \tag{7.18}$$

Furthermore, we can note that in the limit $\Delta t\to 0$, such that $t=n\Delta t$ we have,

$$\lim_{\Delta t\to 0}\frac{\psi_{\Delta t}(n\Delta t)}{\Delta t}=-\frac{d\phi(t)}{dt}=\psi(t), \tag{7.19}$$

where $\psi(t)$ is the probability density associated with the continuous time survival function. The semi-group property of the Markovian survival function can be preserved in the continuous time limit by assuming that there exists a time dependent

hazard rate, $\mu(t)$, such that,

$$\Theta(n,m) = \theta_{\Delta t}(n\Delta t, m\Delta t) = \exp\left(-\int_{m\Delta t}^{n\Delta t} \mu(s)ds\right). \tag{7.20}$$

For the evolving probability function over discrete time we will associate a continuous time function, parameterised by Δt, such that at the points $t = n\Delta t$ we have,

$$x_{\Delta t}(n\Delta t) = X(n), \tag{7.21}$$

and the continuous function is interpolated between these points.

We will also assume that there is a continuous time flux, such that,

$$q_{\Delta t}(n\Delta t) = \frac{Q(n)}{\Delta t} \tag{7.22}$$

To look at the continuous time limit of the discrete equation it is easiest to work from Eq. (7.10). We begin by casting the equation in terms of the newly defined continuous time functions,

$$\begin{aligned} x_{\Delta t}(n\Delta t) - x_{\Delta t}((n-1)\Delta t) = -e^{-\int_0^{n\Delta t}\mu(s)ds} \sum_{k=0}^{n} \Delta t^2 \frac{\psi_{\Delta t}\left((n-k)\Delta t\right)}{\Delta t} \frac{q_{\Delta t}(k\Delta t)}{e^{-\int_0^{k\Delta t}\mu(s)ds}} \\ - \left(1 - e^{-\int_{(n-1)\Delta t}^{n\Delta t}\mu(s)ds}\right) x_{\Delta t}((n-1)\Delta t) + q_{\Delta t}(n\Delta t)\Delta t. \end{aligned} \tag{7.23}$$

Setting $t = n\Delta t$ and expanding the right hand side of this equation about $\Delta t = 0$, whilst noting that,

$$\begin{aligned} \sum_{k=0}^{n} \Delta t^2 \frac{\psi_{\Delta t}\left((n-k)\Delta t\right)}{\Delta t} \frac{q_{\Delta t}(k\Delta t)}{e^{-\int_0^{k\Delta t}\mu(s)ds}} &= \int_0^t \Delta t \frac{\psi_{\Delta t}\left(t-t'\right)}{\Delta t} \frac{q_{\Delta t}(t')}{e^{-\int_0^{t'}\mu(s)ds}} dt' + \mathcal{O}(\Delta t^3) \\ &= \Delta t \int_0^t \psi\left(t-t'\right) \frac{q(t')}{e^{-\int_0^{t'}\mu(s)ds}} dt' + \mathcal{O}(\Delta t^2) \end{aligned} \tag{7.24}$$

then gives,

$$\begin{aligned} x_{\Delta t}(t) - x_{\Delta t}(t-\Delta t) =& q(t)\Delta t - \mu(t)x(t)\Delta t \\ & - e^{-\int_0^t \mu(s)ds}\Delta t \int_0^t \psi\left(t-t'\right) \frac{q(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt' + \mathcal{O}(\Delta t^2). \end{aligned} \tag{7.25}$$

Here we have defined the continuous time limits of $q_{\Delta t}$ and $x_{\Delta t}(n\Delta t)$ such that,

$$\lim_{\Delta t \to 0} q_{\Delta t}(t) = q_0(t) = q(t), \quad \text{and,} \tag{7.26}$$

$$\lim_{\Delta t \to 0} x_{\Delta t}(n\Delta t) = x_0(t) = x(t). \tag{7.27}$$

We now divide both sides of Eq. (7.25) by Δt and take the limit $\Delta t \to 0$ to arrive at the limit equation,

$$\frac{dx(t)}{dt} = q(t) - \mu(t)x(t) - e^{-\int_0^t \mu(s)ds} \int_0^t \psi(t-t') \frac{q(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt'. \tag{7.28}$$

To obtain the continuous time master equation we will rewrite the convolution in Eq. (7.28) via the use of Laplace transforms. Firstly, the continuous time limit of Eq. (7.1) is,

$$x(t)e^{\int_0^t \mu(s)ds} = \int_0^t \phi(t-t')q(t')e^{\int_0^{t'} \mu(s)ds} dt'. \tag{7.29}$$

Similarly to the discrete time case the Laplace transform of this equation can be used to show that,

$$\int_0^t \psi(t-t') \frac{q(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt' = \int_0^t K(t-t') \frac{x(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt', \tag{7.30}$$

where the memory kernel K is defined via its Laplace transform,

$$\mathcal{L}\left\{K(t)\right\} = \frac{\mathcal{L}\left\{\psi(t)\right\}}{\mathcal{L}\left\{\phi(t)\right\}}. \tag{7.31}$$

This then leads to the continuous time master equation,

$$\frac{dx(t)}{dt} = q(t) - \mu(t)x(t) - e^{-\int_0^t \mu(s)ds} \int_0^t K(t-t') \frac{x(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt'. \tag{7.32}$$

This equation is identical to the master equation derived in Angstmann *et al.* [14] for the case of a general compartment model. Given a Mittag-Leffler waiting time distribution, we have,

$$\int_0^t K(t-t') \frac{x(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt' = \tau^{-\alpha} \, {}_0\mathcal{D}_t^{1-\alpha} \left(\frac{x(t')}{e^{-\int_0^{t'} \mu(s)ds}} \right). \tag{7.33}$$

and the general master equation becomes,

$$\frac{dx(t)}{dt} = q(t) - \mu(t)x(t) - \tau^{-\alpha} e^{-\int_0^t \mu(s)ds} \, {}_0\mathcal{D}_t^{1-\alpha} \left(\frac{x(t')}{e^{-\int_0^{t'} \mu(s)ds}} \right), \tag{7.34}$$

which is the general form of the evolution equation for a fractional order compartment model.

7.3.1 Error Analysis

The continuous time limit given above serves to show that the approximation of the continuous time equations by the discrete time stochastic process is convergent. Further to this it would be ideal to have some idea about the accuracy of the approximation. We define the L_1 error in our approximation as,

$$\epsilon_{\Delta t}(t) = |x(t) - x_{\Delta t}(t)|. \tag{7.35}$$

In order to see how this scales with Δt we integrate Eq. (7.28) from $t - \Delta t$ to t,

$$\begin{aligned} x(t) - x(t-\Delta t) = & \int_{t-\Delta t}^t q(u)du - \int_{t-\Delta t}^t \mu(u)x(u)du \\ & - \int_{t-\Delta t}^t e^{-\int_0^u \mu(s)ds} \int_0^u \psi(u-t') \frac{q(t')}{e^{-\int_0^{t'} \mu(s)ds}} dt' du. \end{aligned} \tag{7.36}$$

Taking the series expansion of the right hand side about $\Delta t = 0$ then gives,

$$\begin{aligned} x(t) - x(t-\Delta t) =& q(t)\Delta t - \mu(t)x(t)\Delta t \\ & - e^{-\int_0^t \mu(s)ds}\Delta t \int_0^t \psi(t-t')\frac{q(t')}{e^{-\int_0^{t'} \mu(s)ds}}dt' + \mathcal{O}(\Delta t^2). \end{aligned} \tag{7.37}$$

From Eqs. (7.25) and (7.37) we then find,

$$\epsilon_{\Delta t}(t) = |x(t-\Delta t) - x_{\Delta t}(t-\Delta t) + \mathcal{O}(\Delta t^2)|. \tag{7.38}$$

Hence,

$$\epsilon_{\Delta t}(t) \leq \epsilon_{\Delta t}(t-\Delta t) + \mathcal{O}(\Delta t^2). \tag{7.39}$$

As we have fixed $t = n\Delta t$, we can recursively use this to write,

$$\epsilon_{\Delta t}(t) \leq \epsilon_{\Delta t}(0) + n\mathcal{O}(\Delta t^2). \tag{7.40}$$

Finally noting that our initial condition is exact, and hence $\epsilon_{\Delta t}(0) = 0$, and that n scales with $\frac{1}{\Delta t}$, we find the error bound by a term of order Δt,

$$\epsilon_{\Delta t}(t) \leq \mathcal{O}(\Delta t). \tag{7.41}$$

7.3.2 Stability

In the above subSection we showed that the discrete time process will converge to the continuous time process, and we identified the rate of that convergence. It still remains to be shown that the discrete time process well approximates the continuous time process at some non-infinitesimal Δt. To achieve this we will examine the stability of the approximation. The approximation of the continuous time solution by the discrete time solution will be considered stable if the error remains bounded as $t \to \infty$.

Due to the construction of the continuous time equations from a stochastic process, see Angstmann *et al* [14], the solution must always remain positive, and hence $x(t) \geq 0$ for all t. This is also true for the discrete time solution and is readily seen from Eq. (7.1). First note that $0 \leq \Xi(n,k) \leq 1$ as it is a probability, and $Q(k) > 0$ by construction. From this we see that $X(n) \geq 0$ for all n as it is a sum of non-negative numbers, and then by it definition $x_{\Delta t}(t) \geq 0$. From Eq. (7.35) then we see that,

$$\epsilon_{\Delta t}(t) \leq x(t) + x_{\Delta t}(t), \tag{7.42}$$

and $\epsilon_{\Delta t}$ only diverges if either $x_{\Delta t}$ or x diverge.

Considering the case where we have no additional flux entering the compartment after some time, i.e. $Q(m) = 0$ for all m greater then some number n. In this case $x_{\Delta t}(m\Delta t)$, the solution to the discrete time equations, is a decreasing sequence for all $m > n$. This can be seen from Eq. (7.10), where under these conditions all the terms on the right hand side are negative. Given that $x_{\Delta t}$ is both decreasing and bound non-negative we know that it must be approaching some limit, i.e.,

$$\lim_{m\to\infty} x_{\Delta t}(m\Delta t) = L, \tag{7.43}$$

where the value of L may be dependent on the initial conditions. As such we see that the error is bounded and therefore the solution is stable. Further to this we say that the approximation is unconditionally stable as this stability is independent of the time step size, Δt. The general case of $Q(m) > 0$ is more nuanced as the continuous solution may itself diverge, and this needs to be considered on a case by case basis.

7.4 Multiple Compartments

Thus far we have been concerned about the dynamics of a single compartment. Most compartment models involve a sequence of compartments and as such we need to be able to solve a system of multiple compartments. In an M compartment model each

compartment will have its own survival function, Ξ_i. In addition to this we define an adjacency flux matrix, of size $(M+1)\times(M+1)$, as $\mathbf{Q}(n) = Q_{i,j}(n)$ to describe the flux from compartment i to compartment j at time n. The additional dimension of $\mathbf{Q}(n)$ allows us to capture flux moving in and out of the model that does not originate or terminate in any compartment. The total flux out of compartment i is then the sum over the ith row of $\mathbf{Q}(n)$ and similarly the total flux into compartment i is the sum over the ith column of $\mathbf{Q}(n)$.

Using this notation for the flux and waiting time survival function we may then explicitly define the dynamics of the mass for compartment i using a generalisation of Eq. (7.1),

$$X_i(n) = \sum_{k=0}^{n} \Xi_i(n,k) \sum_{l=1}^{M+1} Q_{l,i}(k). \tag{7.44}$$

Similar to Eq. (7.2) we will assume that the survival functions, Ξ_i are separable into Markovian and non-Markovian survival functions. Further to this we will assume that the Markovian survival function can be separated into survival functions for each Markovian outflow such that,

$$\Xi_i(n,k) = \prod_{j=1}^{M+1} \Theta_{i,j}(n,k)\Phi_{i,j}(n-k). \tag{7.45}$$

Here $\Theta_{i,j}$ is the Markovian survival function for the process in compartment i that will send mass to compartment j, and $\Phi_{i,j}$ is the non-Markov survival function for the process from i to j. Note that we are restricted to a single non-Markov outflow for each compartment, and so $\Phi_{i,j}(n-k) = 1$ for all other compartments.

Further to this we can write Eq. (7.6), in terms of the elements of $\mathbf{Q}$ highlighting its form as a flux balance equation,

$$X_i(n) = X_i(n-1) + \underbrace{\sum_{l=1}^{M+1} Q_{l,i}(n)}_{\text{flux into } X_i} - \underbrace{\sum_{l=1}^{M+1} Q_{i,l}(n)}_{\text{flux out of } X_i}. \tag{7.46}$$

The flux out of the compartment, in terms of the overall survival functions, can be written,

$$\sum_{l=1}^{M+1} Q_{i,l}(n) = \sum_{k=0}^{n-1} \left(\prod_{j=1}^{M+1} \Theta_{i,j}(n-1,k)\Phi_{i,j}(n-1-k) - \prod_{j=1}^{M+1} \Theta_{i,j}(n,k)\Phi_{i,j}(n-k) \right) \times \left(\sum_{l=1}^{M+1} Q_{l,i}(k) \right) \tag{7.47}$$

The decomposition of the right hand side into a sum in order to identify the individual $Q_{i,l}$ from the right hand side is again not unique and will depend on a ordering or the removal processes. Assuming that a particle may only leave the compartment due to Markov process i if it has first survived all Markov processes j, such that $j < i$, and that any non-Markov removal process will alway be considered after the Markov processes, we may write,

$$\begin{aligned} Q_{i,l}(n) = &\sum_{k=0}^{n-1} \left(\prod_{j=1}^{M+1} \Theta_{i,j}(n-1,k)\Phi_{i,j}(n-1-k) \right) (1 - \Theta_{i,l}(n,n-1)) \prod_{j=1}^{l-1} \Theta_{i,j}(n,n-1) \\ &\times \left(\sum_{h=1}^{M+1} Q_{h,i}(k) \right) + \sum_{k=0}^{n-1} \prod_{j=1}^{M+1} \Theta_{i,j}(n,k) \left(\Phi_{i,l}(n-1-k) - \Phi_{i,l}(n-k) \right) \left(\sum_{h=1}^{M+1} Q_{h,i}(k) \right) \end{aligned} \tag{7.48}$$

In going from Eq. (7.47) to Eq. (7.48) it has been assumed that $\Phi_{i,l}(n) = 1$ for all but one l, i.e. there is at most one non-Markovain transition out of each compartment. This is also a requirement so that the continuous time limit will contain fractional derivatives. In the cases where the mass leaving one compartment arrives into another compartment unchanged, then $\mathbf{Q}(n)$ is symmetric and can be recursively constructed via Eq. (7.48). In other cases the flux into the compartments will need to be constructed from the model itself, but Eq. (7.48) will still hold true for the flux out of a compartment. An example of an asymmetric system is provided in Section 7.6.2.

7.5 Implementation

Here we will demonstrate how the discrete time stochastic process can be used as a numerical scheme to solve a fractional-order compartment model. From Eq. (7.44) it is clear that if we know the matrix $\mathbf{Q}$ at all times then we can easily calculate the solution of the fractional order model. The flux, $\mathbf{Q}$, may itself be found via recursion from Eq. (7.48) or similar. The process of constructing this numerical scheme from a given set of equations or block diagram is clearly illustrated by way of example. We will consider the diagram shown in Figure 7.1 and the associated system of equations,

$$\begin{aligned}\frac{dx_1}{dt} = &\underbrace{\lambda(t)}_{\text{flux entering system}} + \underbrace{\left(\tau_2^{-\alpha_2}\theta_2(t)\ {}_0\mathcal{D}_t^{1-\alpha_2}\left(\frac{x_2(t)}{\theta_2(t)}\right) + \beta_2(t)x_2(t)\right)}_{\text{flux in from 2}} \\ &- \underbrace{\left(\tau_1^{-\alpha_1}\theta_1(t)\ {}_0\mathcal{D}_t^{1-\alpha_1}\left(\frac{x_1(t)}{\theta_1(t)}\right) + \beta_1(t)x_1(t)\right)}_{\text{flux out from 1 to 2}}, \end{aligned} \tag{7.49}$$

$$\begin{aligned}\frac{dx_2}{dt} = &\underbrace{\left(\tau_1^{-\alpha_1}\theta_1(t)\ {}_0\mathcal{D}_t^{1-\alpha_1}\left(\frac{x_1(t)}{\theta_1(t)}\right) + \beta_1(t)x_1(t)\right)}_{\text{flux in from 1}} \\ &- \underbrace{\left(\tau_2^{-\alpha_2}\theta_2(t)\ {}_0\mathcal{D}_t^{1-\alpha_2}\left(\frac{x_2(t)}{\theta_2(t)}\right) + \beta_2(t)x_2(t)\right)}_{\text{flux out from 2 to 1}} - \underbrace{\mu(t)x_2(t)}_{\text{flux leaving system}}. \end{aligned} \tag{7.50}$$

Here, $\theta_1(t) = \exp\left(-\int_0^t \beta_1(\tau)d\tau\right)$, and $\theta_2(t) = \exp\left(-\int_0^t \beta_2(\tau) + \mu(\tau)d\tau\right)$. We note that these equations may be nonlinear as λ, β_1, β_2, and μ, are arbitrary time dependent variables and may depend on x_1 and x_2 themselves. These equations will be subject to initial conditions such that $x_1(0) = a$, and $x_2(0) = b$.

The numerical scheme comprises two major parts. To obtain an approximation for $x_1(t)$ and $x_2(t)$, we will first calculate $\mathbf{Q}(m)$ for all $m < n$ such that $t = n\Delta t$. Following this we will calculate X_1 and X_2 via Eq. (7.44) and use these to form our approximation. To do this we will need to relate the discrete parameters and probabilities to the known parameters given in the continuous time equations. The

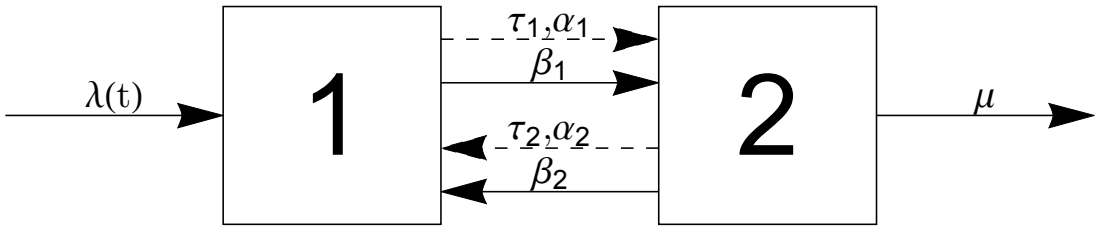

Figure 7.1: Box diagram for the case considered in the implementation Section. The solid arrows indicate a Markovian transition from one compartment to another with a rate parameter indicated above the arrow. Arrows originating or terminating on no compartment indicate transitions in and out of the system respectively. Dashed arrow indicate a non-Markovian transition with the first parameter above the arrow being a time scale and the second parameter being the exponent.

discrete time process is completely described by the survival functions and incoming flux. Considering compartment 1 the Markov survival function is,

$$\Theta_{1,2}(n,m) = \exp\left(-\int_{m\Delta t}^{n\Delta t} \beta_1(\tau)d\tau\right), \tag{7.51}$$

and the non-Markov survival function is,

$$\Phi_{1,2}(n) = E_{\alpha_1,1}\left(-\left(\frac{n\Delta t}{\tau_1}\right)^{\alpha_1}\right). \tag{7.52}$$

Note that this non-Markov survival function is chosen so that in the limit $\Delta t \to 0$ we will recover the Mittag-Leffler survival function, Eq. (3.39), that leads to the fractional derivative appearing in the continuum equations. The discrete time flux entering compartment 1 from outside the system can be found from,

$$Q_{3,1}(n) = \int_{(n-1)\Delta t}^{n\Delta t} \lambda(\tau)d\tau + a\delta_{n,0}. \tag{7.53}$$

where $\delta_{n,0}$ is a Kronecker Delta function and the term $a\delta_{n,0}$ is used to establish the initial condition. In compartment 2 we have two Markovian out processes and one

non-Markov out process. The Markov survival functions are,

$$\Theta_{2,1}(n,m) = \exp\left(-\int_{m\Delta t}^{n\Delta t} \beta_2(\tau)d\tau\right), \tag{7.54}$$

and

$$\Theta_{2,3}(n,m) = \exp\left(-\int_{m\Delta t}^{n\Delta t} \mu(\tau)d\tau\right). \tag{7.55}$$

The non-Markov survival function is

$$\Phi_{2,1}(n) = E_{\alpha_2,1}\left(-\left(\frac{n\Delta t}{\tau_2}\right)^{\alpha_2}\right). \tag{7.56}$$

Compartment 2 does not have any flux entering from outside the system and so the flux $Q_{3,2}$ will only incoporate the initial condition,

$$Q_{3,2}(n) = b\delta_{n,0}. \tag{7.57}$$

The flux matrix that we wish to compute then is,

$$\mathbf{Q}(n) = \begin{pmatrix} 0 & Q_{1,2} & 0 \\ Q_{2,1} & 0 & Q_{2,3} \\ Q_{3,1} & Q_{3,2} & 0 \end{pmatrix}. \tag{7.58}$$

We know $Q_{3,1}$ via Eq. (7.53) and $Q_{3,2}$ via Eq. (7.57), leaving only three matrix elements that must be calculated recursively. Starting with the flux entering compartment 1 from compartment 2 we have, from Eq.(7.48),

$$\begin{aligned} Q_{2,1}(n) = &\sum_{k=0}^{n-1} \Theta_{2,1}(n,k)\Theta_{2,3}(n,k)(\Phi_{2,1}(n-1-k) - \Phi_{2,1}(n-k))(Q_{1,2}(k) + Q_{3,2}(k)) \\ &+ \sum_{k=0}^{n-1} \Theta_{2,1}(n-1,k)\Theta_{2,3}(n-1,k)\Phi_{2,1}(n-1-k)(1-\Theta_{2,1}(n,n-1))(Q_{1,2}(k) + Q_{3,2}(k)). \end{aligned} \tag{7.59}$$

Similarly, using Eq. (7.48), we find the flux entering compartment 2 from compartment 1,

$$\begin{aligned} Q_{1,2}(n) = &\sum_{k=0}^{n-1} \Theta_{1,2}(n-1,k)\Phi_{1,2}(n-1-k)(1-\Theta_{1,2}(n,n-1))(Q_{2,1}(k)+Q_{3,1}(k)) \\ &+ \sum_{k=0}^{n-1} \Theta_{1,2}(n,k)(\Phi_{1,2}(n-1-k)-\Phi_{1,2}(n-k))(Q_{2,1}(k)+Q_{3,1}(k)). \end{aligned} \tag{7.60}$$

Lastly, using Eq. (7.48), the flux leaving the system from compartment 2 is,

$$\begin{aligned} Q_{2,3}(n) = \sum_{k=0}^{n-1} &\Theta_{2,1}(n,k)\Theta_{2,3}(n-1,k)\Phi_{2,1}(n-1-k)(1-\Theta_{2,3}(n,n-1)) \\ &\times(Q_{1,2}(k)+Q_{3,2}(k)). \end{aligned} \tag{7.61}$$

Finally, to obtain the approximation we use Eq. (7.46),

$$x_{1\Delta t}(n\Delta t) = X_1(n) = X_1(n-1) + Q_{2,1}(n) + Q_{3,1}(n) - Q_{1,2}(n), \tag{7.62}$$

$$x_{2\Delta t}(n\Delta t) = X_2(n) = X_2(n-1) + Q_{1,2}(n) + Q_{3,2}(n) - Q_{2,1}(n) - Q_{2,3}(n). \tag{7.63}$$

7.6 Examples

Here we consider a collection of examples that have been chosen for their tractability, enabling us to make comparisons with exact solutions. The fractional derivative in all these examples ensures that the evolution has a dependence on the entire history, and thus includes a non-local memory effect.

7.6.1 A Single Compartment Model for Chromium Poisoning

We consider a one-compartment model describing the clearance of chromium in mice considered in Subsection 3.4.2 [14]. This compartment model comprises of a single compartment that has an initial dose of chromium, c_0, that exits out of the compartment via a non-Markovian process, see Figure 7.2.

The amount of chromium in the compartment, $c(t)$, changes according to the fractional order DE,

$$\frac{dc}{dt} = -\tau^{\alpha}\ {}_0D_t^{1-\alpha}c(t), \tag{7.64}$$

where τ is a time scale and α the exponent, subject to the initial condition $c(0) = c_0$. The exact solution to Eq. (7.64) is given by,

$$c(t) = c_0 E_{\alpha,1}\left(-(\tau t)^{\alpha}\right). \tag{7.65}$$

Using our discrete time stochastic process this governing equation can be approximated by its discrete time analog. As outlined in Section 7.5, we will come about this approximation by considering the flux for the system. As there is a single compartment we will consider a two dimensional flux matrix,

$$\mathbf{Q} = \begin{pmatrix} 0 & Q_{1,2} \\ Q_{2,1} & 0 \end{pmatrix}, \tag{7.66}$$

where $Q_{2,1}(n)$ is the flux into the compartment and $Q_{1,2}$ is the flux out of the compartment. The only flux into the compartment, $Q(k)$, is the initial dosage and hence we may write,

$$Q_{2,1}(n) = c_0\delta_{n,0}, \tag{7.67}$$

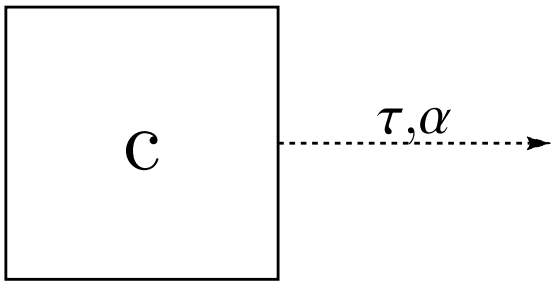

Figure 7.2: A one compartment model for the clearance of chromium. There is a single non-Markovian transition out of the compartment with time scale τ and exponent α.

where $\delta_{n,0}$ is the Kronecker delta function and c_0 is the initial dosage concentration. The non-Markovian survival function is given by

$$\Phi_{1,2}(n) = E_{\alpha,1}\left(-\left(\tau n \Delta t\right)^{\alpha}\right), \tag{7.68}$$

and there are no Markovian processes. Hence, from Eq. (7.48), we can write,

$$Q_{1,2}(n) = \sum_{k=0}^{n-1} (\Phi_{1,2}(n-1-k) - \Phi_{1,2}(n-k))(Q_{2,1}(k)). \tag{7.69}$$

Substituting Eq. (7.67) into this gives,

$$Q_{1,2}(n) = c_0(\Phi_{1,2}(n-1) - \Phi_{1,2}(n)), \tag{7.70}$$

for $n \geq 1$. Finally our approximation for the solution is found from Eq. (7.46),

$$c_{\Delta t}(n\Delta t) = X_1(n) = X_1(n-1) - c_0(\Phi_{1,2}(n-1) - \Phi_{1,2}(n)), \tag{7.71}$$

for $n \geq 1$ and $X(0) = c_0$. This recursive relation can be solved to give,

$$c_{\Delta t}(n\Delta t) = X_1(n) = c_0 E_{\alpha,1}\left(-\left(\tau n \Delta t\right)^{\alpha}\right). \tag{7.72}$$

Hence in this case our numerical approximation gives the exact solution at discrete points, $t = n\Delta t$.

7.6.2 Two Compartment Model for in Host HIV Dynamics

HIV has been the subject of numerous mathematical models, typically aiming to describe the population dynamics of the virus itself and the CD4+ T cells, targeted by the virus [119]. We consider a simplistic two-compartment model describing these dynamics in the case of a combined antiretroviral therapy with 100% efficacy, leading to no replenishment of the infected T-cells from uninfected cells. This model has

been considered in it's continuum in Subsection 3.4.3 [14]. The model is governed by

$$\frac{dI}{dt} = -\delta_I^{\alpha}\, {}_0\mathcal{D}_t^{1-\alpha}\, I, \tag{7.73}$$

and

$$\frac{dV}{dt} = N\delta_I^{\alpha}\, {}_0\mathcal{D}_t^{1-\alpha}\, I - \delta_V V, \tag{7.74}$$

where I denotes the number of infected CD4+ T cells and V the number of HIV virons, subject to the initial conditions,

$$I(0) = I_0, \tag{7.75}$$

$$V(0) = V_0. \tag{7.76}$$

The solution of these equations is given by [14],

$$I(t) = I_0 E_{\alpha,1}\left(-(\delta_I t)^{\alpha}\right). \tag{7.77}$$

$$\begin{aligned} V(t) =& e^{-\delta_V t} I_0 N \left(\left[1 - e^{\delta_V t} E_{\alpha,1}\left(-(\delta_I t)^{\alpha}\right)\right] + \delta_V \int_0^t e^{\delta_V s} E_{\alpha,1}\left(-(\delta_I s)^{\alpha}\right)\, ds \right) \\ &+ V_0 e^{-\delta_V t} \end{aligned} \tag{7.78}$$

In representing this as a compartment model, we consider three compartments, with I is taken to be the first compartment, V to be the second, and a third dummy compartment for outflows an initial inflows. This is illustrated schematically in Figure 7.3).

The flux matrix $\mathbf{Q}(n)$ for this example is given by

$$\mathbf{Q} = \begin{pmatrix} 0 & 0 & Q_{1,3} \\ 0 & 0 & Q_{2,3} \\ Q_{3,1} & Q_{3,2} & 0 \end{pmatrix}. \tag{7.79}$$

The flux into the I compartment from the dummy compartment is used to give the initial condition such that,

$$Q_{3,1}(n) = I_0 \delta_{n,0}, \tag{7.80}$$

From the model we see that the flux into the V compartment from the dummy compartment is a multiple of the flux out of the I compartment into the dummy compartment, plus our initial condition term. Hence we can write,

$$Q_{3,2}(n) = N Q_{1,3}(n) + V_0 \delta_{n,0}. \tag{7.81}$$

This just leaves the flux out of each compartment into the dummy compartment. A single non-Markov process removes particles from the I compartment, from Eq. (7.48) we can therefore write,

$$Q_{1,3}(n) = \sum_{k=0}^{n-1} (\Phi_{1,3}(n-1-k) - \Phi_{1,3}(n-k))(Q_{3,1}(k)), \tag{7.82}$$

with

$$\Phi_{1,3}(n) = E_{\alpha,1}\left(-\left(\delta_I n \Delta t\right)^{\alpha}\right). \tag{7.83}$$

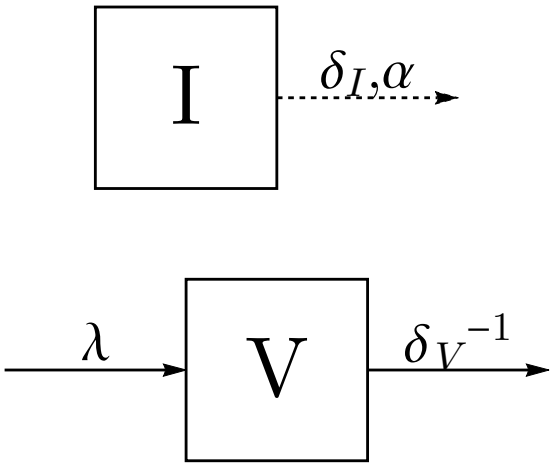

Figure 7.3: Diagram for the HIV model. Here the Infected cells die with a non-Markovian transition. The virions grow proportionally to the death of the Infected cells, such that $\lambda = N \delta_I^{\alpha}\, {}_0\mathcal{D}_t^{1-\alpha}\, I$, and themselves are cleared via a Markov transition.

Using Eq. (7.80), this becomes,

$$Q_{1,3}(n) = I_0(\Phi_{1,3}(n-1) - \Phi_{1,3}(n)), \tag{7.84}$$

and Eq. (7.81) becomes,

$$Q_{3,2}(n) = NI_0(\Phi_{1,3}(n-1) - \Phi_{1,3}(n)) + V_0\delta_{n,0}. \tag{7.85}$$

Lastly we have the flux from the V compartment to the dummy compartment, which again can be found from Eq. (7.48),

$$Q_{2,3}(n) = \sum_{k=0}^{n-1}(\Theta_{2,3}(n-1,k) - \Theta_{2,3}(n-k))Q_{3,2}(k). \tag{7.86}$$

Here the Markovian survival function can be constructed from the continuous time parameters such that,

$$\Theta_{2,3}(n,m) = \exp\left(-\int_{m\Delta t}^{n\Delta t} \delta_V d\tau\right). \tag{7.87}$$

Our approximation can then be found by considering Eq. (7.46),

$$I_{\Delta t}(n\Delta t) = X_1(n) = X_1(n-1) + Q_{3,1}(n) - Q_{1,3}(n), \tag{7.88}$$

$$V_{\Delta t}(n\Delta t) = X_2(n) = X_2(n-1) + Q_{3,2}(n) - Q_{2,3}(n). \tag{7.89}$$

Again, we can note that the recursion equation for $I_{\Delta t}(n\Delta t)$, can be solved so that,

$$I_{\Delta t}(n\Delta t) = I_0 E_{\alpha,1}\left(-\left(\delta_I n\Delta t\right)^{\alpha}\right), \tag{7.90}$$

and our numerical approximation gives the exact solution for $I(t)$ at discrete points, $t = n\Delta t$. However the numerical approximation for $V(t)$ will not be exact.

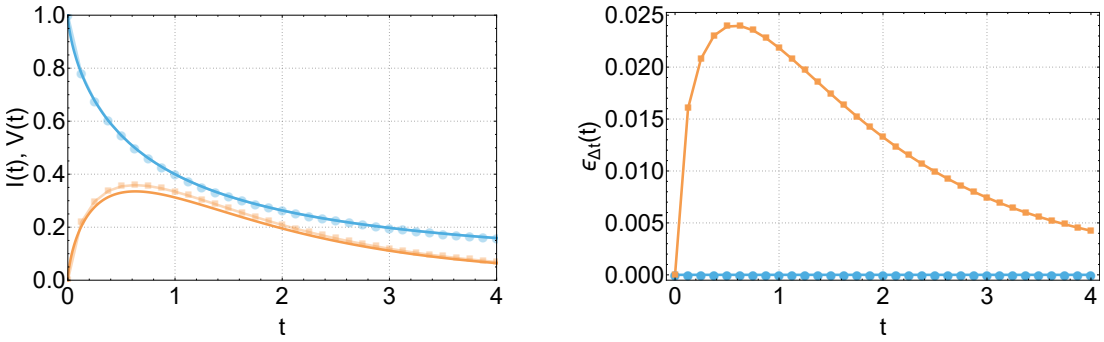

Figure 7.4: Left: Comparison of approximate DTRW solution for I compartment ($\circ$) and V compartment ($\square$) against exact solutions (solid line). Right: L_1 error in approximate DTRW solution for I compartment ($\circ$) and V compartment ($\square$). Plots are given on the domain $t \in [0, 4]$, with $\alpha = 0.7$ and $\Delta t = 1/8$.

Figure 7.4 illustrates a comparison between the exact solution and the numerical solution obtained by the present method with $V_0 = 0$, $I_0 = 1$, $\delta_I = 1$, $\delta_V = 1$, $\Delta t = 1/8$ and $\alpha = 0.7$. A coarse grid has been taken to exaggerate the difference between these solutions in the $V(t)$ compartment. The error shown in Figure 7.4 is problem specific and will grow or shrink depending on the problem dynamics. In Figure 7.5 the L_1 error in the numerical approximation of $V(t)$ has been plotted as a function of Δt, with $V_0 = 0$, $I_0 = 1$, $\delta_I = 1$, $\delta_V = 1$. Since our numerical solution is evaluated at discrete points, $n\Delta t$, we choose the evaluation time ($t = 0.4$) such that t is an integer number of Δt steps. For Figure 7.5 we used $\Delta t = 0.4/2^j$ for $j = 0, 1, \ldots, 9$. The error for three values of α have been plotted and all show the linear relationship as expected by Eq. (7.41).

7.6.3 Two Compartment Model with Fractional Feedback

We now consider a two compartment model with a non-Markovian feedback loop, as seen in Figure 7.6. This dynamic is captured by,

$$\frac{dx}{dt} = \delta^\alpha \, {}_0\mathcal{D}_t^{1-\alpha}(y - x) \tag{7.91}$$

$$\frac{dy}{dt} = \delta^\alpha \, {}_0\mathcal{D}_t^{1-\alpha}(x - y) \tag{7.92}$$

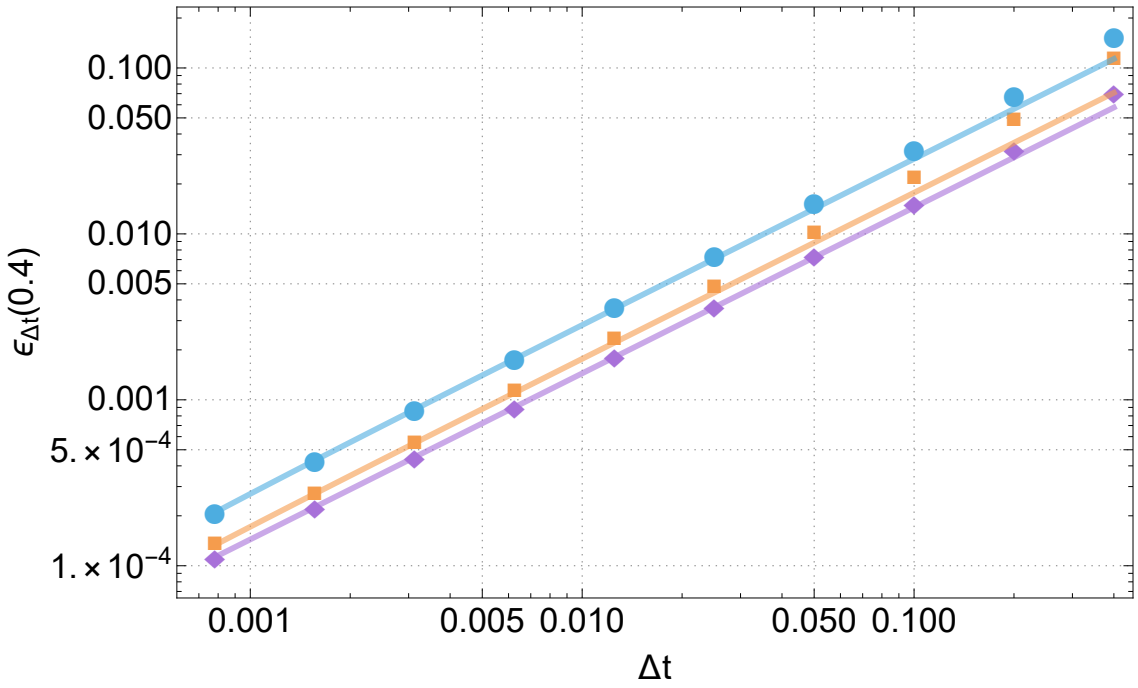

Figure 7.5: Plot of the convergence of the L_1 error for the numerical approximation of the concentration in the V compartment at $t = 0.4$ over Δt for $\alpha = 0.1$ ($\circ$), $\alpha = 0.5$ ($\square$) and $\alpha = 0.9$ ($\diamond$).

with initial conditions $x(0) = x_0$ and $y(0) = y_0$. The exact solution for this system is given by,

$$x(t) = \frac{1}{2}\left((x_0 - y_0)E_{\alpha,1}(-2\delta^\alpha t^\alpha) + x_0 + y_0\right) \tag{7.93}$$

$$y(t) = \frac{1}{2}\left((y_0 - x_0)E_{\alpha,1}(-2\delta^\alpha t^\alpha) + x_0 + y_0\right) \tag{7.94}$$

The numerical approximation will again be constructed by considering the flux out of each compartment. Identifying compartment x as 1, and y as 2, the flux matrix for the DTRW is,

$$\mathbf{Q} = \begin{pmatrix} 0 & Q_{1,2} & 0 \\ Q_{2,1} & 0 & 0 \\ Q_{3,1} & Q_{3,2} & 0 \end{pmatrix}. \tag{7.95}$$

The flux from the dummy compartment to each of the other two compartment encodes the initial condition so that,

$$Q_{3,1}(n) = x_0\delta_{n,0}, \tag{7.96}$$

and

$$Q_{3,2}(n) = y_0\delta_{n,0}. \tag{7.97}$$

The other two fluxes are both due to non-Markovian processes and there are no Markovian processes present. As such we can use Eq. (7.48) to write,

$$Q_{1,2}(n) = \sum_{k=0}^{n-1} \left(\Phi_{1,2}(n-1-k) - \Phi_{1,2}(n-k)\right)\left(Q_{2,1}(k) + Q_{3,1}(k)\right), \tag{7.98}$$

and

$$Q_{2,1}(n) = \sum_{k=0}^{n-1} \left(\Phi_{2,1}(n-1-k) - \Phi_{2,1}(n-k)\right)\left(Q_{1,2}(k) + Q_{3,2}(k)\right). \tag{7.99}$$

Comparison with the continuous time equations give the non-Markkov survival functions as,

$$\Phi_{1,2}(n) = \Phi_{2,1}(n) = E_{\alpha,1}\left(-\left(\delta n\Delta t\right)^{\alpha}\right). \tag{7.100}$$

The numerical approximation can then be constructed from Eq. (7.46) giving,

$$x_{\Delta t}(n\Delta t) = X_1(n) = X_1(n-1) + Q_{3,1}(n) + Q_{2,1}(n) - Q_{1,2}(n) \tag{7.101}$$

$$y_{\Delta t}(n\Delta t) = X_2(n) = X_2(n-1) + Q_{3,2}(n) + Q_{1,2}(n) - Q_{2,1}(n) \tag{7.102}$$

We numerically consider the above system subject to $x_0 = 1$ and $y_0 = 0$. Figure 7.7 illustrates a comparison between the exact solution and the numerical solution obtained by the present method with $\Delta t = 1/8$, $\delta = 1$, and $\alpha = 0.7$. We again choose a coarse grid to exaggerate the difference between these solutions in the $x(t)$ and $y(t)$ compartments. Due to the symmetry of the problem the errors in the $x(t)$ and

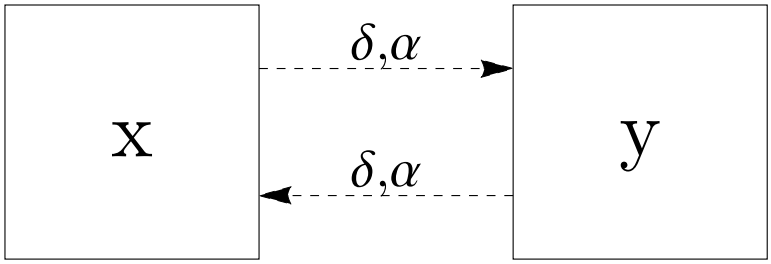

Figure 7.6: Diagram for two compartment fractional feedback loop. In this case there are identical non-Markovian transitions between each of the compartments and no Markovian transitions.

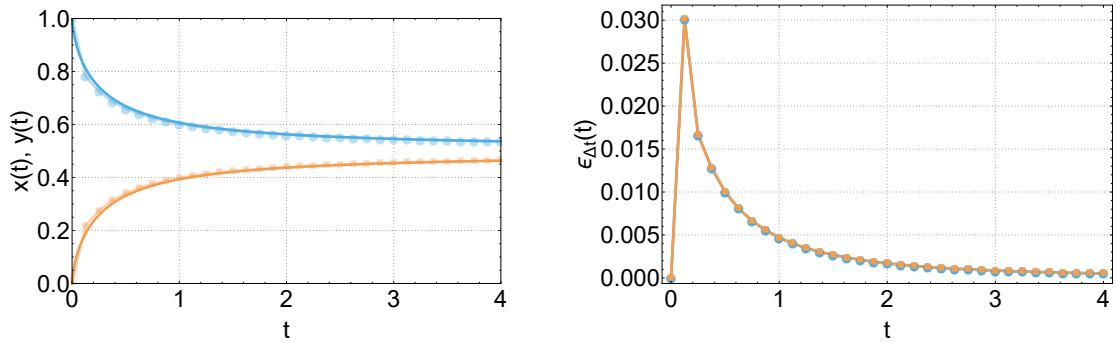

Figure 7.7: Left: Comparison of approximate DTRW solution for x compartment ($\circ$) and y compartment ($\square$) against exact solutions (solid line). Right: L_1 error in approximate DTRW solution for x compartment ($\circ$) and y compartment ($\square$). Plots are given on the domain $t \in [0, 4]$, with $\alpha = 0.7$ and $\Delta t = 1/8$.

$y(t)$ solutions are identical. Figure 7.8 plots the L_1 error of the solution as a function of Δt for a range of α values. Once again the slope of the curve indicates that Eq. (7.41) holds. We note that the analysis conducted in Section 7.3.2, specifically Eq. (7.41), provides asymptotic behaviour of the error as $\Delta t \to 0$. As such the errors reported in Figure 7.8 deviate from the theoretical bounds for large Δt.

7.7 Summary

We have developed a new numerical method for solving a class of coupled fractional order differential equations that arise in modelling with compartment models. This method, developed by considering an underlying stochastic process, is robust and easy to implement. The method is unconditionally stable, in the sense that arbitrarily large time steps can be taken, which is advantageous at small α values

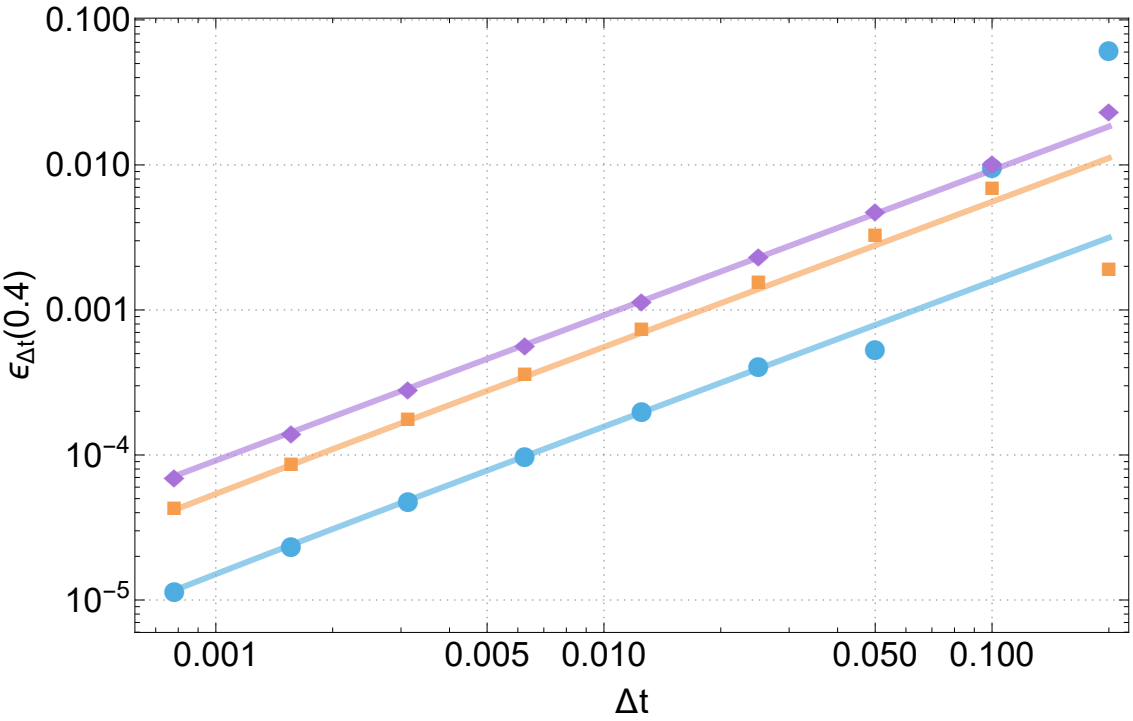

Figure 7.8: Plot of the convergence of the L_1 error for the numerical approximation of the concentration in the x compartment at $t = 0.4$ over Δt for $\alpha = 0.1$ ($\circ$), $\alpha = 0.5$ ($\square$) and $\alpha = 0.9$ ($\diamond$). Note that due to the symmetry of the problem the L_1 error for the x compartment is equal to the L_1 error for the y compartment.

where more traditional methods, such as finite difference methods based on the Grünwald-Letnikov derivative become unstable with larger time steps [134]. Examples of various compartment models were considered. In each case the results are in agreement with our analysis.

The procedure for obtaining a numerical method that we have developed can be applied when there is a known underlying stochastic process for the fractional DEs. It is interesting to speculate if more general fractional DEs could be derived from a stochastic process in which case the procedure could be applied more generally. As an example we recently derived a fractional advection equation, without diffusion, from a stochastic process [18], featured in the following Chapter. Another interesting area to pursue is that different stochastic processes may limit to the same fractional DEs [11, 18] and thus would produce distinct numerical schemes. It therefore may be

possible to find a more optimal numerical scheme by considering different stochastic processes.

Part II

Fractional-Order PDE Models

Chapter 8

Fractional Advection Equation without Diffusion

8.1 Introduction

This Chapter moves away from the ODE space of the first Part of this thesis and presents a derivation for a fractional-order PDE. We have derived a time fractional partial differential advection equation by considering an advective limit in the generalized master equations for CTRWs on a one dimensional lattice with power-law distributed waiting times. This follows the publication [18]. We have also derived the generalized master equations for corresponding DTRWs which limit to the same fractional advection equation and we use these master equations as a basis for obtaining numerical approximations to the solutions of the fractional advection equation.

The remainder of this chapter is as follows: In Section 8.2 we derive the generalized master equations for CTRWs on a one-dimensional lattice, with a power-law waiting time density and with two different jump length densities - a two-sided density, and a one-sided density. We derive a fractional Fokker-Planck equation from the diffusive limit of the master equation, and a fractional generalized advection equation from an advective limit of the master equation. In Section 8.3 we derive the generalized master equations for DTRWs on a one-dimensional lattice with a power-law waiting time probability mass function and with two different jump length densities. We show that the fractional generalized advection equation is recovered

in an advective limit. In Section 8.4 we consider two different numerical approximations for the solution of the fractional advection equation, one based on the DTRW master equation with a two-sided jump length density and the other based on the DTRW master equation with a one-sided jump length density. This is illustrated with an example. We conclude with a summary in Section 8.5.

8.2 The Master Equation of a CTRW

The CTRW on a one-dimensional lattice is a stochastic process in which a particle resides on a lattice site for some random amount of time, drawn from a waiting time probability density function, before jumping to a site on the lattice governed by a jump length probability density. The stochastic CTRW process has been widely employed in derivations of fractional Fokker-Planck type equations [28, 142, 61, 7, 11]. There are two fundamental steps in these derivations. The first is the derivation of the generalized master equation that governs the time evolution of the probability density for the location of the particle. The second is taking the diffusive limit of the generalized master equation to obtain a partial differential equation.

For completeness, we revisit the derivation of the generalized master equation. We also include the consideration of two different jump length densities; a two-sided density, and a one-sided density. We then consider different limits to fractional partial differential equations; a diffusive limit and an advective limit.

To begin, we consider a one-dimensional lattice with sites denoted by x_i where $i \in \mathbb{N}$. The flux of probability of the particle entering the lattice site x_i at time t, after having taken n jumps can be defined recursively by,

$$q_{n+1}(x_i, t) = \sum_j \int_0^t \Psi(x_i, t|x_j, t') q_n(x_j, t') dt', \tag{8.1}$$

where $\Psi(x_i, t|x_j, t')$ is the transition probability density for a particle that arrived at lattice site x_j at time t' to jump to lattice site x_i at time t. As Ψ is independent

of n, the number of jumps taken, we may write the flux entering lattice site x_i, unconditional on n, as,

$$q(x_i, t) = \sum_{n=0}^{\infty} q_n(x_i, t). \tag{8.2}$$

The flux entering the lattice site x_i after any number of steps can then by written recursively as,

$$q(x_i, t) = q_0(x_i, t) + \sum_j \int_0^t \Psi(x_i, t|x_j, t')q(x_j, t')dt'. \tag{8.3}$$

In the following we suppose that Ψ is separable such that,

$$\Psi(x_i, t|x_j, t') = \lambda(x_i, t|x_j)\psi(t - t'). \tag{8.4}$$

Here ψ is a waiting time density that governs how long the particle will stay at the site, and λ a jump length density that governs the length of the jump. The jump length density is normalised such that,

$$\sum_i \lambda(x_i, t|x_j) = 1, \tag{8.5}$$

and the waiting time density is normalised as,

$$\int_0^{\infty} \psi(t)dt = 1. \tag{8.6}$$

In the case where the particle begins at a lattice site, x_0, at time $t = 0$, the initial flux condition will be a product of a Kronecker and a Dirac delta functions, i.e. $q_0(x_i, t) = \delta_{x_i,x_0}\delta(t)$. Other initial conditions have been considered recently in [24]. For the subsequent derivation, we split the flux into the discontinuous and differentiable components, i.e.,

$$q(x_i, t) = \delta_{x_i,x_0}\delta(t) + q^+(x_i, t), \tag{8.7}$$

where the differentiable component is given by,

$$q^+(x_i,t) = \sum_j \int_0^t \lambda(x_i,t|x_j)\psi(t-t')q(x_j,t')dt'. \tag{8.8}$$

The master equation governs the evolution of the probability density, $\rho(x_i,t)$, for the position of the particle. This probability density is related to the flux, via

$$\rho(x_i,t) = \int_0^t \Phi(t-t')q(x_i,t')dt', \tag{8.9}$$

where Φ is the survival function associated with the waiting time density. The survival function can be computed from the waiting time density,

$$\Phi(t) = 1 - \int_0^t \psi(t')dt'. \tag{8.10}$$

To obtain the master equation we first differentiate Eq. (8.9) to give,

$$\begin{aligned}\frac{\partial\rho(x_i,t)}{\partial t} &= q^+(x_i,t) - \int_0^t \psi(t-t')q(x_i,t')dt', \\ &= \sum_j \int_0^t \lambda(x_i,t|x_j)\psi(t-t')q(x_j,t')dt' - \int_0^t \psi(t-t')q(x_i,t')dt'.\end{aligned} \tag{8.11}$$

It remains to express the right hand side of this equation in terms of ρ. This can be achieved by introducing a memory kernel $K(t)$ with the property that

$$\int_0^t \psi(t-t')q(x_i,t')dt' = \int_0^t K(t-t')\rho(x,t')dt'. \tag{8.12}$$

An explicit representation of the memory kernel can be obtained using Laplace transform methods. We use the notation

$$\mathcal{L}_t\{g(x,t)\} = \int_0^\infty e^{-st}g(x,t)dt. \tag{8.13}$$

for the Laplace transform from t to s and $\mathcal{L}_s^{-1}$ as the inverse Laplace transform from s to t. We now take the Laplace transforms of Eq. (8.9) and of Eq. (8.12) using the convolution theorem, and we combine the results to obtain the Laplace transform of the memory kernel,

$$\mathcal{L}_t\{K(t)\} = \frac{\mathcal{L}_t\{\psi(t)\}}{\mathcal{L}_t\{\Phi(t)\}} \tag{8.14}$$

and then the memory kernel is given by,

$$K(t) = \mathcal{L}_s^{-1}\left\{\frac{\mathcal{L}_t\{\psi(t)\}}{\mathcal{L}_t\{\Phi(t)\}}\right\}, \tag{8.15}$$

The master equation for the CTRW is now simply found by substituting Eq. (8.12) into Eq. (8.11). This yields

$$\begin{aligned}\frac{\partial\rho(x_i,t)}{\partial t} &= \sum_j \lambda(x_i,t|x_j)\int_0^t K(t-t')\rho(x_j,t')dt' - \int_0^t K(t-t')\rho(x_i,t')dt', \\ &= \sum_j \left(\lambda(x_i,t|x_j) - \delta_{x_i,x_j}\right)\int_0^t K(t-t')\rho(x_j,t')dt'.\end{aligned} \tag{8.16}$$

8.2.1 Mittag-Leffler Waiting Time Density and Fractional Derivatives

The master equation derived above is valid for any waiting time density. If a heavy tailed waiting time density is chosen, then the master equation may be expressed with fractional-order derivatives [67, 106]. Again we consider a Mittag-Leffler waiting time density with the survival function,

$$\Phi(t) = E_\alpha\left(-\left(\frac{t}{\tau}\right)^\alpha\right), \tag{8.17}$$

where E_α is a one parameter Mittag-Leffler function defined by,

$$E_\alpha(t) = \sum_{k=0}^{\infty}\frac{t^k}{\Gamma(\alpha k+1)}. \tag{8.18}$$

The memory kernel corresponding to the Mittag-Leffler waiting time density is,

$$K(t) = \mathcal{L}_s^{-1}\left\{\frac{s^{1-\alpha}}{\tau^\alpha}\right\}. \tag{8.19}$$

This memory kernel allows us to write,

$$\begin{aligned}\int_0^t K(x_i, t-t')\rho(x_i,t')dt' &= \mathcal{L}_s^{-1}\left\{\mathcal{L}_t\{K(x_i,t)\}\mathcal{L}_t\{\rho(x_i,t)\}\right\}, \\ &= \mathcal{L}_s^{-1}\left\{\frac{s^{1-\alpha}}{\tau^\alpha}\mathcal{L}_t\{\rho(x_i,t)\}\right\}.\end{aligned} \tag{8.20}$$

As discussed in Section 2.3, the inverse Laplace transform can be carried out, resulting in a time fractional-order derivative. For $0 < \alpha < 1$, we have,

$$\int_0^t K(x_i, t-t')\rho(x_i,t')dt' = \frac{1}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t). \tag{8.21}$$

Substituting the relation in Eq. (8.21) into Eq. (8.16), gives the master equation for a CTRW with Mittag-Leffler distributed waiting times,

$$\frac{\partial\rho(x,t)}{\partial t} = \sum_{x'}\left(\lambda(x,t|x') - \delta_{x,x'}\right)\tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x',t). \tag{8.22}$$

We show below that depending on the choice of jump length density, and the particular limit in which it is considered, this master equation can be the basis for the fractional Fokker-Planck equation as well as the fractional advection equation.

8.2.2 Two-Sided Jump Length Density

Firstly, we will consider a two-sided biased nearest neighbour jump length density,

$$\lambda(x_i,t|x_j) = p_r(x_j,t)\delta_{x_j,x_{i-1}} + p_l(x_j,t)\delta_{x_j,x_{i+1}}, \tag{8.23}$$

where $p_r(x_i,t)$, and $p_l(x_i,t)$, are the probability to jump to the right, and left, from site x_i given that the jump occurs at time t. Substituting this into Eq. (8.22) gives,

$$\begin{aligned}\frac{\partial\rho(x_i,t)}{\partial t} =&\frac{p_r(x_{i-1},t)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i-1},t)+\frac{p_l(x_{i+1},t)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i+1},t)\\ &-\frac{1}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_i,t).\end{aligned}\tag{8.24}$$

It is convenient to exploit the normalisation condition $p_r(x_i,t)+p_l(x_i,t)=1$ and write,

$$p_r(x_i,t)=\frac{1}{2}+\frac{1}{2}f(x_i,t),\quad\text{and}\quad p_l(x_i,t)=\frac{1}{2}-\frac{1}{2}f(x_i,t),\tag{8.25}$$

where $f(x_i,t)=p_r(x_i,t)-p_l(x_i,t)$. Equation (8.24) can now be written as,

$$\begin{aligned}&\frac{\partial\rho(x_i,t)}{\partial t}=\frac{1}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i-1},t)+\frac{1}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i+1},t)\\ &-\frac{1}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_i,t)+\frac{f(x_{i-1},t)}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i-1},t)-\frac{f(x_{i+1},t)}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i+1},t).\end{aligned}\tag{8.26}$$

In order to obtain a spatially continuous equation we will consider limits such that the lattice spacing, Δx, goes to zero. In Eq. (8.26), we write $x_i=x$ and $x_{i\pm1}=x\pm\Delta x$, giving,

$$\begin{aligned}&\frac{\partial\rho(x,t)}{\partial t}=\frac{1}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x-\Delta x,t)+\frac{1}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x+\Delta x,t)\\ &-\frac{1}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)+\frac{f(x-\Delta x,t)}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x-\Delta x,t)-\frac{f(x+\Delta x,t)}{2\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x+\Delta x,t).\end{aligned}\tag{8.27}$$

Prior to considering limits as $\Delta x\to0$, we take the Taylor expansion of the terms in Eq. (8.26), about $\Delta x=0$. This gives,

$$\frac{\partial\rho(x,t)}{\partial t}=-\frac{\partial}{\partial x}\left(f(x,t)\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right)\frac{\Delta x}{\tau^\alpha}+\frac{\partial^2}{\partial x^2}\left({}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right)\frac{\Delta x^2}{2\tau^\alpha}+\mathcal{O}(\Delta x^3).\tag{8.28}$$

There are two ways in which we can take the limit $\Delta x\to0$ in Eq. (8.28) in which the terms remain finite.

8.2.2.1 Diffusive Limit

A diffusive limit is taken by considering the case where both the lattice spacing, Δx, and the waiting time scale, τ, are taken to zero such that the limit,

$$D_\alpha = \lim_{\Delta x, \tau \to 0} \frac{\Delta x^2}{2\tau^\alpha}, \tag{8.29}$$

exists. In order for the first term on the right hand side of Eq. (8.28) to remain finite under such a limit, we let $f(x,t)$ scale with Δx and be $\mathcal{O}(\Delta x)$. Using Eq. (8.29) and introducing another function,

$$F(x,t) = \lim_{\Delta x \to 0} \frac{f(x,t)}{\Delta x}, \tag{8.30}$$

we can take the limit $\Delta x \to 0$ in Eq. (8.28) to arrive at the fractional Fokker-Planck equation,

$$\frac{\partial \rho(x,t)}{\partial t} = -2D_\alpha \frac{\partial}{\partial x}\left(F(x,t)\, {}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right) + D_\alpha \frac{\partial^2}{\partial x^2}\left({}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right). \tag{8.31}$$

8.2.2.2 Advective Limit

An advective limit can be taken by considering the case where, $f(x,t)$ has no Δx dependence and the lattice spacing, Δx, and the waiting time scale, τ, are taken to zero such that the limit,

$$C_\alpha = \lim_{\Delta x, \tau \to 0} \frac{\Delta x}{\tau^\alpha}, \tag{8.32}$$

exists. In this case, in the limit $\Delta x \to 0$, we arrive at the fractional generalised advection equation,

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(v(x,t)\, {}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right), \tag{8.33}$$

where $v(x,t) = C_\alpha f(x,t)$ is interpreted as the advective velocity. As $f(x,t)$ is bound between $[-1,1]$ the advective velocity is bound between $[-C_\alpha, C_\alpha]$.

8.2.3 One-Sided jump length density

An alternative approach to arrive at a fractional generalised advection equation from a CTRW master equation is by considering a one-sided jump length density. Without loss of generality we consider a right-moving random walk with jump length density given by,

$$\lambda(x_i, t|x_j) = p_s(x_j, t)\delta_{x_j,x_i} + p_r(x_j, t)\delta_{x_j,x_{i-1}}. \tag{8.34}$$

Here $p_s(x_i, t)$ is the probability to jump back to the same site at x_i given that a jump occurs at time t. Substituting this jump length density into Eq. (8.22) gives,

$$\frac{\partial\rho(x_i,t)}{\partial t} = \frac{p_r(x_{i-1},t)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_{i-1},t) - \frac{p_r(x_i,t)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x_i,t). \tag{8.35}$$

As in the case of the two sided jump length density, in order to take the continuous limit we write $x_i = x$ and $x_{i-1} = x - \Delta x$,

$$\frac{\partial\rho(x,t)}{\partial t} = \frac{p_r(x-\Delta x,t)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x-\Delta x,t) - \frac{p_r(x,t)}{\tau^\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t), \tag{8.36}$$

where we have made use of the normalisation $p_r(x,t) + p_s(x,t) = 1$.

Taking a Taylor expansion with respect to Δx, around $\Delta x = 0$ of the terms on the right hand side of Eq. (8.36), we have,

$$\begin{aligned}\frac{\partial\rho(x,t)}{\partial t} = &-\frac{\partial}{\partial x}\left(p_r(x,t)\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right)\frac{\Delta x}{\tau^\alpha} \\ &+\frac{\partial^2}{\partial x^2}\left(p_r(x,t)\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right)\frac{\Delta x^2}{2\tau^\alpha} + \mathcal{O}\left(\Delta x^3\right).\end{aligned} \tag{8.37}$$

Here, in contrast to the two-sided jump length density, we are only able to take an advective limit. This is due to the appearance of p_r in the first two terms on the right hand side of Eq. (8.37), so that any scaling of p_r with Δx would be redundant.

8.2.3.1 Advective Limit

In a similar manner to the advective limit taken with the two-sided jump length density, we again take a limit as Δx and τ go to zero such that C_α exists. This yields,

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(u(x,t)\,{}_0\mathcal{D}_t^{1-\alpha}\rho(x,t)\right), \tag{8.38}$$

where,

$$u(x,t) = C_\alpha p_r(x,t), \tag{8.39}$$

and $u(x,t)$ is bound between zero and C_α.

We note that in the advective limit, both the one- and two-sided jump length densities, yield an equivalent fractional generalised advection equation. However, the one-sided jump length density is unable to produce a fractional Fokker-Planck equation as the diffusive limit of the generalised master equation does not exist except in the most trivial case.

8.3 Discrete Formulation

In this section we derive a discrete time form of the time-fractional advection equation. We show that this discrete scheme limits to the time-fractional partial differential equation derived in Section 8.2 and go on to illustrate how the discrete form may be used as a numerical scheme for simulating the equation's dynamics.

We begin by considering the motion of a particle on an arbitrary lattice $\{\ldots, x_{i-1}, x_i, x_{i+1}, \ldots\}$ at some discrete time $n \in \mathbb{N}$. We define a transition probability distribution, $\Psi(x_j, n|x_i, m)$, which dictates the probability of the particle moving from site x_i at time m to site x_j at a later time n. We assume that the transition probability distribution is separable into independent waiting time, $\psi(n-m)$, and jump, $\lambda(x_j, n|x_i)$, distributions such that,

$$\Psi(x_j, n|x_i, m) = \lambda(x_j, n|x_i)\psi(n-m). \tag{8.40}$$

The probability distribution functions are normalised so that,

$$\sum_{n=0}^{\infty} \psi(n) = 1 \tag{8.41}$$

and

$$\sum_{j=-L}^{j=L} \lambda(x_j, n|x_i) = 1. \tag{8.42}$$

The flux of probability of the particle entering the lattice site x_i at time step n having taken w jumps can be recursively defined as

$$Q_{w+1}(x_i, n) = \sum_{j} \sum_{n=0}^{n-1} \Psi(x_i, n|x_j, m) Q_w(x_j, m). \tag{8.43}$$

As Ψ is independent of the number of jumps taken we may write the total probability flux as,

$$Q(x_i, n) = \sum_{w=0}^{\infty} Q_w(x_i, n). \tag{8.44}$$

Summing over w on both side of Eq. (8.43) then gives,

$$Q(x_i, n) = Q_0(x_i, n) + \sum_{j} \sum_{n=0}^{n-1} \Psi(x_i, n|x_j, m) Q(x_j, m), \tag{8.45}$$

where $Q_0(x_i, n)$ is the initial condition term, for example when the particle begins at lattice site x_0 at $n = 0$ then $Q_0(x_i, n) = \delta_{x_i,x_0}\delta_{n,0}$. The probability of waiting from time m to n without jumping is given by,

$$\Phi(n - m) = 1 - \sum_{k=0}^{n-m} \psi(k), \tag{8.46}$$

and hence the probability of a particle being at a site x_i after the n^{th} time step is,

$$X(x_i, n) = \sum_{m=0}^{n} \Phi(n - m) Q(x_i, m). \tag{8.47}$$

This can be interpreted as the collection of probability mass that has jumped to a site x_i at all previous time steps and not jumped away by time step n. Implicitly, we have $X(x_i, n) = 0$ for $n < 0$ from our taken initial condition.

Subtracting $X(x_i, n-1)$ from each side of Eq. (8.47) gives,

$$X(x_i, n) - X(x_i, n-1) = Q(x_i, n) - \sum_{m=0}^{n-1} \psi(n-m) Q(x_i, m). \tag{8.48}$$

Substituting Eq. (8.45) into Eq. (8.48), we obtain,

$$\begin{aligned} X(x_i, n) - X(x_i, n-1) = Q_0(x_i, n) + \sum_j \lambda(x_i, n|x_j) \sum_{n=0}^{n-1} \psi(n-m) Q(x_j, m) \\ - \sum_{m=0}^{n-1} \psi(n-m) Q(x_i, m). \end{aligned} \tag{8.49}$$

We now seek a memory kernel through which we may obtain the generalised master equation (GME). In an analogous fashion to the CTRW, we begin by taking the single sided Z-transform, defined by

$$\hat{Y}(z) = \mathcal{Z}_n\{Y(n)\} = \sum_{n=0}^{\infty} Y(n) z^{-n}, \tag{8.50}$$

of Eq. (8.47) which yields

$$\hat{X}(x_i, z) = \hat{\Phi}(z) \hat{Q}(x_i, z). \tag{8.51}$$

We define a discrete memory kernel as

$$\hat{K}(z) = \frac{\hat{\psi}(z)}{\hat{\Phi}(z)}, \tag{8.52}$$

noting that $K(0) = 0$. Through the inverse Z-transform we may now arrive at the relation

$$\sum_{m=0}^{n-1} \psi(n-m) Q(x, m) = \sum_{m=0}^{n-1} K(n-m) X(x, m). \tag{8.53}$$

This result is readily verified by taking the Z-transform of both sides and using Eqs. (8.51) and (8.52). Using this result we may write Eq. (8.49) in terms of probability mass $X(x_i, n)$ which gives the GME,

$$X(x_i, n) - X(x_i, n-1) = \sum_{x_j} \left(\lambda(x_i, n|x_j) - \delta_{x_i,x_j}\right) \sum_{m=0}^{n-1} K(n-m)X(x_j, m), \quad (8.54)$$

for $n > 0$ and assuming that the particle began at $n = 0$.

8.3.1 Sibuya Waiting Time Distribution

The above master equation is valid for any discrete waiting time density. In order to obtain fractional-order time derivatives in the limit we will need to consider a heavy tailed waiting time density. We will consider Sibuya distributed waiting times [139], whose probability mass function is given by,

$$\psi(n) = \frac{\alpha}{n} \prod_{k=1}^{n-1} (1 - \frac{\alpha}{k}). \quad (8.55)$$

The survival function is,

$$\phi(n) = \prod_{k=1}^{n-1} (1 - \frac{\alpha}{k}). \quad (8.56)$$

It is straight forward to write down the memory kernel for the Sibuya distribution from Eq. (8.52). First noting that,

$$\mathcal{Z}_n\{\psi(n)\} = 1 - (1 - z^{-1})^{\alpha}, \quad (8.57)$$

and

$$\mathcal{Z}_n\{\phi(n)\} = (1 - z^{-1})^{\alpha-1}, \quad (8.58)$$

we find

$$K(n) = \delta_{1,n} + \prod_{k=1}^{n} \left(1 - \frac{2-\alpha}{k}\right), \quad (8.59)$$

for $n > 0$, and $K(0) = 0$.

8.3.2 Two-sided jump distribution

In a similar manner to the continuous time case we will first consider a two-sided biased nearest neighbour jump length density,

$$\lambda(x_i, n|x_j) = p_r(x_j, n)\delta_{x_j,x_{i-1}} + p_l(x_j, n)\delta_{x_j,x_{i+1}}. \tag{8.60}$$

where $p_r(x_i, n)$ and $p_l(x_i, n)$ are the probabilities to jump to the right and left from site x_i given that the jump occurs on time step n. Substituting this into Eq. (8.54), together with Eq. (8.59), gives for $n > 0$,

$$\begin{aligned} X(x_i, n) =& p_r(x_{i-1}, n)\left(X(x_{i-1}, n-1) + \sum_{m=0}^{n-1}\prod_{k=1}^{n-m}\left(1 - \frac{2-\alpha}{k}\right)X(x_{i-1}, m)\right) \\ &+ p_l(x_{i+1}, n)\left(X(x_{i+1}, n-1) + \sum_{m=0}^{n-1}\prod_{k=1}^{n-m}\left(1 - \frac{2-\alpha}{k}\right)X(x_{i+1}, m)\right) \\ &- \sum_{m=0}^{n-1}\prod_{k=1}^{n-m}\left(1 - \frac{2-\alpha}{k}\right)X(x_i, m). \end{aligned} \tag{8.61}$$

The diffusive limit of this master equation is a fractional Fokker-Planck equation, for details see [13, 9]. As such we will examine the advective limit.

8.3.2.1 Advective Limit

Unlike the continuous time case, the continuum limits are difficult to calculate directly. As such we will follow the method outlined in [9] and approach the limits via Z- and Laplace transforms.

We associate a function in continuous space and time to our discrete space and time functions via the limit of a Z-star transform. The unilateral Z-star transform from n to s also depends on a scale parameter Δt, and is defined by,

$$\mathcal{Z}_n^*\left\{Y(x_i, n)\right\} = \sum_{n=0}^{\infty} Y(x_i, n)e^{-n\Delta t s}. \tag{8.62}$$

We will also make use of a bilateral Z-star transform over the spatial lattice. With a lattice spacing of Δx, such that $x_i = i\Delta x$, from x_i to q this transform is defined by,

$$\mathcal{Z}_i^* \{Y(x_i, n)\} = \sum_{i=-\infty}^{\infty} Y(i\Delta x, n) e^{-i\Delta x q}. \tag{8.63}$$

For an arbitrary function, $Y(x_i, n)$, in discrete time and space we define the continuous limit of the function as,

$$y(x,t) = \lim_{\Delta x \to 0, \Delta t \to 0} \Delta x \Delta t \mathcal{L}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \mathcal{Z}_i^* \left\{ \mathcal{Z}_n^* \left\{ Y(x_i, n) \right\} \right\} \right\} \right\}. \tag{8.64}$$

Under this process it can be shown [9] that the continuous limit of the product of two discrete functions is the product of the continuous limits, i.e.,

$$y_1(x,t) y_2(x,t) = \lim_{\Delta x \to 0, \Delta t \to 0} \Delta x \Delta t \mathcal{L}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \mathcal{Z}_i^* \left\{ \mathcal{Z}_n^* \left\{ Y_1(x_i, n) Y_2(x_i, n) \right\} \right\} \right\} \right\}. \tag{8.65}$$

The shift relations for the Z-star transforms are,

$$\mathcal{Z}_n^* \{Y(x_i, n-k)\} = e^{-k\Delta t s} \mathcal{Z}_n^* \{Y(x_i, n)\}, \tag{8.66}$$

$$\mathcal{Z}_i^* \{Y(x_{i-k}, n)\} = e^{-k\Delta x q} \mathcal{Z}_n^* \{Y(x_i, n)\}. \tag{8.67}$$

It is convenient to adopt the notation,

$$\hat{Y}_\Delta(q,s) = \mathcal{Z}_i^* \left\{ \mathcal{Z}_n^* \left\{ Y(x_i, n) \right\} \right\}. \tag{8.68}$$

In the same manner as the continuous time case we define the function,

$$F(x_i, n) = p_r(x_i, n) - p_l(x_i, n). \tag{8.69}$$

This allows us to write the master equation, Eq. (8.54) as,

$$X(x_i,n) - X(x_i,n-1) - Q_0(x_i,n) = \frac{1}{2}\sum_{m=0}^{n-1} K(n-m)X(x_{i-1},m)$$
$$+ \frac{1}{2}\sum_{m=0}^{n-1} K(n-m)X(x_{i+1},m) - \frac{1}{2}\sum_{m=0}^{n-1} K(n-m)X(x_i,m)$$
$$+ \frac{F(x_{i-1},n)}{2}\sum_{m=0}^{n-1} K(n-m)X(x_{i-1},m) - \frac{F(x_{i+1},n)}{2}\sum_{m=0}^{n-1} K(n-m)X(x_{i+1},m). \tag{8.70}$$

Taking the Z-star transform of this equation then gives,

$$(1-e^{-s\Delta t})\hat{X}_\Delta(q,s) - \hat{Q}_0(q,s) = \frac{1}{2}\left(e^{-q\Delta x} + e^{q\Delta x} - 2\right)\hat{K}_\Delta(s)\hat{X}_\Delta(q,s)$$
$$+ (e^{-q\Delta x} - e^{q\Delta x})\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{\frac{F(x_i,n)}{2}\sum_{m=0}^{n-1} K(n-m)X(x_i,m)\right\}\right\} \tag{8.71}$$

Multiplying the left hand side by $\frac{\Delta x\Delta t}{\Delta t}$ and the right hand side by $\frac{\Delta x^2\Delta t}{\Delta x\Delta t}$ and taking the inverse Laplace transforms we will arrive at our continuous time and space limit. All limits will be considered such that $t = n\Delta t$, $x = i\Delta x$, and,

$$C_\alpha = \lim_{\Delta t,\Delta x\to 0}\frac{\Delta x}{\Delta t^\alpha}. \tag{8.72}$$

Firstly the limit for the left hand side is easily calculated,

$$\lim_{\Delta x,\Delta t\to 0}\Delta x\Delta t\mathcal{L}_s\left\{\mathcal{L}_q\left\{\frac{(1-e^{-s\Delta t})\hat{X}_\Delta(q,s) - \hat{Q_{0\Delta}}(q,s)}{\Delta t}\right\}\right\} = \frac{\partial u(x,t)}{\partial t}, \tag{8.73}$$

where we have defined,

$$u(x,t) = \lim_{\Delta x\to 0,\Delta t\to 0}\Delta x\Delta t\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{X(x_i,n)\right\}\right\}\right\}\right\}, \tag{8.74}$$

and used the fact that,

$$\lim_{\Delta x,\Delta t\to 0}\frac{\Delta x\Delta t}{\Delta t}\mathcal{L}_s\left\{\mathcal{L}_q\left\{\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{Q_0(x_i,n)\right\}\right\}\right\}\right\}=u(x,0). \tag{8.75}$$

The next limit we need to consider is also straightforward to calculate,

$$\lim_{\Delta x,\Delta t\to 0}\mathcal{L}_s\left\{\mathcal{L}_q\left\{\frac{\Delta x^2\Delta t^{\frac{1}{2}}\left(e^{-q\Delta x}+e^{q\Delta x}-2\right)\hat{K}_\Delta(s)\hat{X}_\Delta(q,s)}{\Delta x\Delta t}\right\}\right\}=0. \tag{8.76}$$

It should be noted that under a diffusive limit this would be non-zero and contribute the second order spatial derivative.

Lastly we need to calculate,

$$\begin{aligned}W=\lim_{\Delta x,\Delta t\to 0}\frac{\Delta x^2\Delta t}{\Delta t}\mathcal{L}_s\left\{\mathcal{L}_q\left\{\left(\frac{e^{-q\Delta x}-e^{q\Delta x}}{2\Delta x}\right)\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{F(x_i,n)\right.\right.\right.\right.\\ \left.\left.\left.\left.\times\sum_{m=0}^{n-1}K(n-m)X(x_i,m)\right\}\right\}\right\}\right\}.\end{aligned} \tag{8.77}$$

Which is equivalent to,

$$W=-\frac{\partial}{\partial x}\left(\lim_{\Delta x,\Delta t\to 0}\frac{\Delta x^2\Delta t}{\Delta t}\mathcal{L}_s\left\{\mathcal{L}_q\left\{\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{F(x_i,n)\sum_{m=0}^{n-1}K(n-m)X(x_i,m)\right\}\right\}\right\}\right\}\right). \tag{8.78}$$

Making use of the property given in Eq. (8.65), and the definition from Eq. (8.72), this can be written as,

$$W=-\frac{\partial}{\partial x}\left(f(x,t)\lim_{\Delta x,\Delta t\to 0}\frac{\Delta x\Delta t}{\Delta t^{1-\alpha}}\mathcal{L}_s\left\{\mathcal{L}_q\left\{\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{\sum_{m=0}^{n-1}K(n-m)X(x_i,m)\right\}\right\}\right\}\right\}\right). \tag{8.79}$$

where we have defined,

$$f(x,t)=\lim_{\Delta x\to 0,\Delta t\to 0}C_\alpha\Delta x\Delta t\mathcal{L}_q^{-1}\left\{\mathcal{L}_s^{-1}\left\{\mathcal{Z}_i^*\left\{\mathcal{Z}_n^*\left\{F(x_i,n)\right\}\right\}\right\}\right\}. \tag{8.80}$$

The Z-star transform of the Sibuya memory kernel, Eq. (8.59), is,

$$\mathcal{Z}_n^* \{K(n)\} = \left(1 - e^{-s\Delta t}\right)^{1-\alpha} - \left(1 - e^{-s\Delta t}\right) = (s\Delta t)^{1-\alpha} + \mathcal{O}(\Delta t). \tag{8.81}$$

Using this in Eq. (8.79) gives,

$$W = -\frac{\partial}{\partial x}\left(f(x,t) \lim_{\Delta x, \Delta t \to 0} \frac{\Delta x \Delta t}{\Delta t^{1-\alpha}} \mathcal{L}_s \left\{ \mathcal{L}_q \left\{ \left(\left(1 - e^{-s\Delta t}\right)^{1-\alpha} - \left(1 - e^{-s\Delta t}\right) \right) \hat{X}_\Delta(q,s) \right\} \right\}\right). \tag{8.82}$$

Finally taking the limit and noting the Laplace transform of the Riemann-Liouville fractional derivative, Eq. (2.59) we arrive at,

$$W = -\frac{\partial}{\partial x}\left(f(x,t)\, {}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right)\right). \tag{8.83}$$

From this we see that the advective continuum limit of the master equation with Sibuya waiting times is,

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(f(x,t)\, {}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right)\right). \tag{8.84}$$

This is identical to the advective continuum limit of the CTRW master equation with Mittag-Leffler distributed waiting times.

8.3.3 One-sided jump distribution

Again similar to the continuous time case we will consider a right moving one sided jump length density given by,

$$\lambda(x_i, n|x_j) = p_r(x_j, n)\delta_{x_j, x_{i-1}} + p_s(x_j, n)\delta_{x_j, x_i}, \tag{8.85}$$

where $p_s(x_i, n)$ is the probability of a length zero jump back to the same site given that the jump occurs on time step n. Substituting this into Eq. (8.54), together

with Eq. (8.59), gives for $n > 0$,

$$\begin{aligned} X(x_i,n) =& p_r(x_{i-1},n)\left(X(x_{i-1},n-1)+\sum_{m=0}^{n-1}\prod_{k=1}^{n-m}\left(1-\frac{2-\alpha}{k}\right)X(x_{i-1},m)\right) \\ &- p_r(x_i,n)\left(X(x_i,n-1)+\sum_{m=0}^{n-1}\prod_{k=1}^{n-m}\left(1-\frac{2-\alpha}{k}\right)X(x_i,m)\right) \\ &+ X(x_i,n-1)+Q_0(x_i,n). \end{aligned} \tag{8.86}$$

In the same manner as the two-sided jump distribution we can find the continuum limit of this master equation by first considering the Z-transform,

$$(1-e^{-s\Delta t})\hat{X}_\Delta(q,s)-\hat{Q_{0\Delta}}(q,s) = (e^{-q\Delta x}-1)Z_n^*\left\{Z_i^*\left\{p_r(x_i,n)\sum_{m=0}^{n-1}K(m-n)X(x_i,m)\right\}\right\}. \tag{8.87}$$

Multiplying the left hand side by $\frac{\Delta x\Delta t}{\Delta t}$ and the right hand side by $\frac{\Delta x^2\Delta t}{\Delta x\Delta t}$, the advective continuum limit is found by taking the inverse Laplace transform of the equation and the limit as Δx and Δt go to zero such that Eq. (8.72) holds, with $x = i\Delta x$, and $t = n\Delta t$. The limit of the left hand side is again straight forward,

$$\lim_{\Delta x,\Delta t\to 0}\Delta x\Delta t\mathcal{L}_s\left\{\mathcal{L}_q\left\{\frac{(1-e^{-s\Delta t})\hat{X}_\Delta(q,s)-\hat{Q_{0\Delta}}(q,s)}{\Delta t}\right\}\right\} = \frac{\partial u(x,t)}{\partial t}, \tag{8.88}$$

again using Eqs. (8.74) and (8.75). Using the same method as for the two-sided jump distribution, the limit for the right hand side can also be found,

$$\begin{aligned} &\lim_{\Delta,\Delta t\to 0}\mathcal{L}_t\left\{\mathcal{L}_x\left\{\frac{\Delta x^2\Delta t}{\Delta x\Delta t}(e^{-q\Delta x}-1)Z_n^*\left\{Z_i^*\left\{p_r(x_i,n)\sum_{m=0}^{n-1}K(m-n)X(x_i,m)\right\}\right\}\right\}\right\} \\ &= -\frac{\partial}{\partial x}\left(f(x,t)\,{}_0\mathcal{D}_t^{1-\alpha}\left(u(x,t)\right)\right), \end{aligned} \tag{8.89}$$

where,

$$f(x,t) = \lim_{\Delta x \to 0, \Delta t \to 0} C_\alpha \Delta x \Delta t \mathcal{L}_q^{-1} \left\{ \mathcal{L}_s^{-1} \left\{ \mathcal{Z}_i^* \left\{ \mathcal{Z}_n^* \left\{ p_r(x_i, n) \right\} \right\} \right\} \right\}. \tag{8.90}$$

Hence the advective continuum limit of the DTRW with a one-sided jump distribution and Sibyua distributed waiting times is,

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left(f(x,t) \, {}_0\mathcal{D}_t^{1-\alpha} \left(u(x,t) \right) \right), \tag{8.91}$$

which is identical to both the CTRW and the two-sided jump distribution cases.

8.4 Numerical Approximations

Whilst we have shown that both choices of jump distribution share a limit, we are often interested in how close to the limit we are for some non-zero lattice spacing. This is particularly true for the discrete time and space processes that could be used to obtain numerical approximations.

8.4.1 Exact Solution

In order to compare how close each of the master equations is to the limit we need an exact solution to which we can compare. Here we consider the solution $u(x,t)$ to the fractional advection equation

$$\frac{\partial u}{\partial t} = -\, {}_0D_t^{1-\alpha} \frac{\partial u}{\partial t} \tag{8.92}$$

with the periodic boundaries

$$u(1,t) = u(-1,t) \tag{8.93}$$

and initial condition

$$u(x,0) = 1 - \cos \pi x. \tag{8.94}$$

We seek a separable solution of the form

$$u(x,t) = X(x)T(t) \tag{8.95}$$

which leads to the ordinary differential equations

$$X'(x) = \lambda X(x) \tag{8.96}$$

and

$$T'(t) = -\lambda\, {}_0D_t^{1-\alpha} T(t). \tag{8.97}$$

The solution to the spatial part is trivially found to be

$$X(x) = e^{\lambda x} \tag{8.98}$$

with eigenvalues

$$\lambda = \pm n\pi i \quad n \in \mathbb{N}. \tag{8.99}$$

To find the solution to the temporal part we take the Laplace transform of Eq. (8.97) and solve for

$$\hat{T}(s) = \frac{T(0)s^{\alpha-1}}{s^\alpha + \lambda} \tag{8.100}$$

where $\hat{T}(s)$ denotes the Laplace transform from t to s of $T(t)$. It is a simple matter to invert Eq. (8.100) arriving at

$$T(t) = T(0)E_\alpha(\lambda t^\alpha). \tag{8.101}$$

The zero eigenvalue results in a constant solution, and then, using the results in Eqs. (8.95), (8.98), (8.101), (8.99), the general solution is the linear superposition

$$u(x,t) = C_0 + \sum_{n=1}^{\infty} A_n e^{in\pi x} E_\alpha(-in\pi t^\alpha) + B_n e^{-in\pi x} E_\alpha(in\pi t^\alpha). \tag{8.102}$$

The constants A_n and B_n need to be chosen in such a way that the solution $u(x,t)$ is real valued. To arrive at the real solution we first introduce the two-parameter Mittag-Leffler function [58]

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta + \alpha k)}. \tag{8.103}$$

It is now straightforward, using elementary manipulations on the expressions in Eq. (8.18) and Eq. (8.103), to show that

$$E_{\alpha}(\pm in\pi t^{\alpha}) = E_{2\alpha}(-n^2\pi^2 t^{2\alpha}) \pm in\pi t^{\alpha} E_{2\alpha,1+\alpha}(-n^2\pi^2 t^{2\alpha}). \tag{8.104}$$

We now subsititute the above identity, Eq. (8.104), together with Euler's formula

$$e^{\pm in\pi t^{\alpha}} = \cos(n\pi t^{\alpha}) \pm i \sin(n\pi t^{\alpha}),$$

into Eq. (8.102), and combine terms to write

$$\begin{aligned} u(x,t) = C_0 &+ \sum_{n=1}^{\infty} a_n \left[\cos(n\pi x) E_{2\alpha}(-n^2\pi^2 t^{2\alpha}) + \sin(n\pi x) n\pi t^{\alpha} E_{2\alpha,1+\alpha}(-n^2\pi^2 t^{2\alpha})\right] \\ &- \sum_{n=1}^{\infty} b_n \left[\cos(n\pi x) n\pi t^{\alpha} E_{2\alpha,1+\alpha}(-n^2\pi^2 t^{2\alpha}) - \sin(n\pi x) E_{2\alpha}(-n^2\pi^2 t^{2\alpha})\right] \end{aligned} \tag{8.105}$$

where $a_n = A_n + B_n$ and $b_n = i(A_n - B_n)$ are real valued arbitrary constants to be determined by the initial conditions. Using the initial conditions in Eq. (8.94) we find $C_0 = 1, a_1 = -1, b_1 = 0$ and $a_n = 0, b_n = 0$ for $n \geq 2$. Thus we have the solution

$$u(x,t) = 1 - \cos(\pi x) E_{2\alpha}(-\pi^2 t^{2\alpha}) - \sin(\pi x)\pi t^{\alpha} E_{2\alpha+1,\alpha}(-\pi^2 t^{2\alpha}) \tag{8.106}$$

8.4.2 Comparison

The construction of the DTRW master equation in discrete time and space makes it particularly amenable for numerical approximations. Equations (8.61) and (8.86) can both be used to iterate the probability density forward in time. All that is required is the appropriate selection of parameters such that the advective continuum limit of the master equations matches the exact solution derived above. For the two-sided jump distribution we need values for $p_r(x,t)$, $p_l(x,t)$, Δx, and Δt. From Eqs. (8.69), (8.72), and (8.80), we see that we need to set,

$$\Delta t = \left(\frac{\Delta x}{C_\alpha}\right)^{\frac{1}{\alpha}}, \tag{8.107}$$

and,

$$p_r(x,t) = \frac{1}{2}\left(\frac{1}{C_\alpha} + 1\right). \tag{8.108}$$

Note that here we are using C_α and Δx as free parameters, and setting the value of p_l through the relationship, $p_r + p_l = 1$. The constraint that $0 < p_r < 1$ therefore also constrains the choice of C_α such that $C_\alpha > 1$ and $\Delta x > \Delta t^\alpha$.

Similarly for the one-sided jump distribution we need a values for $p_r(x,t)$, Δx, and Δt. From Eqs. (8.72), and(8.90), we see that we need to set,

$$\Delta t = \left(\frac{\Delta x}{C_\alpha}\right)^{\frac{1}{\alpha}}, \tag{8.109}$$

and,

$$p_r(x,t) = \frac{1}{C_\alpha}. \tag{8.110}$$

To compare the distance that each DTRW is from the exact solution we will use a L_∞ norm and define the distance from the exact solution, for a given Δx and Δt at $t = n\Delta t$, by,

$$L_\infty(X,u) = \max(\{|X(x_i,n) - u(i\Delta x,t)|\}_i), \tag{8.111}$$

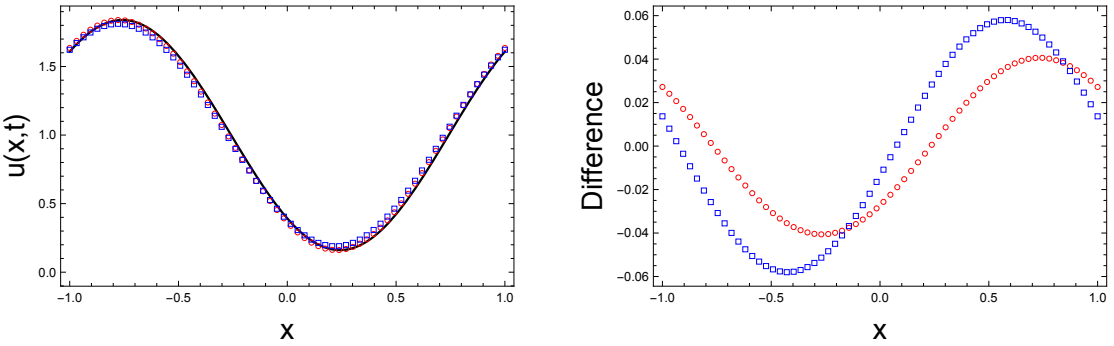

Figure 8.1: Left, Plot of the exact solution, together with the one-sided jump distribution DTRW (red circles) and the two-sided jump distribution DTRW (blue squares). Right, the difference between the exact solution and the one-sided jump distribution DTRW (red circles) and the two-sided jump distribution DTRW (blue squares). Here $\alpha = \frac{1}{2}$, $C_\alpha = 2$, and $\Delta x = \frac{2}{63}$. The solutions are evaluated at $t = \frac{200}{3\sqrt{7}}$.

i.e. the absolute value of the maximum difference between the DTRW and the exact solutions.

In Figure 8.1 a plot of the solution for each of the DTRWs is given, as well as a plot of the difference between each solution and the exact solution. This clearly shows that the one-sided jump distribution results in a DTRW master equations whose solution is closer to the exact solution.

In Figure 8.2, we show how the distance from the exact solution scales with time and Δx for both the DTRWs. Again from this figure it is clear that the one-sided jump distribution produces a solution that is closer to the exact solution across all time and for all values of Δx.

8.5 Summary

The Chapter highlights the practicality of considering continuous time, and discrete time, random walks, and their limit processes, in deriving fractional-order PDEs. Solutions of fractional-order PDEs that are derived in this way are guaranteed to be positive and finite. Moreover the corresponding master equations from the discrete time random walk formulations can be interpreted as stable finite difference approximations to the solutions. In this Chapter we considered the fractional advection equation that is obtained in the advective limit from the generalized master

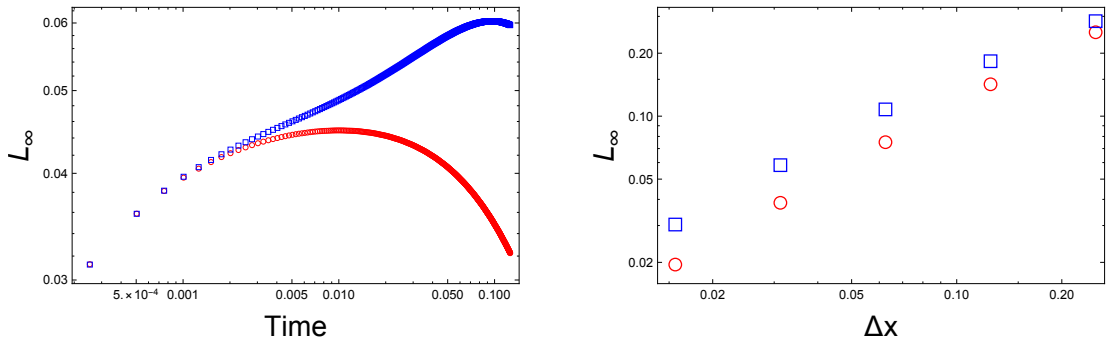

Figure 8.2: Left, L_∞ scaling time for the the one-sided jump distribution DTRW (red circles) and the two-sided jump distribution DTRW (blue squares) with $\Delta x = \frac{2}{63}$. Right, L_∞ vs Δx for the one-sided jump distribution DTRW (red circles) and the two-sided jump distribution DTRW (blue squares) at $t = \frac{1}{16}$. Here $\alpha = \frac{1}{2}$ and $C_\alpha = 2$.

equations of CTRWs and DTRWs, with power-law distributed waiting times, and with two different types of jump densities. In particular we considered a two-sided jump density where the particle could jump in either direction on the lattice and we considered a one-sided jump density where the particle could not jump along one direction. We arrived at the same fractional advection equation in each case, even though the generalized master equations were different. The fact that the master equations for different CTRWs, or different DTRWs may limit to the same fractional-order partial differential equation, provides evidence of the robustness of the limiting partial differential equation as a valid mathematical model. On the other hand, the different master equations provide different choices on a DTRW based numerical scheme, as presented in the previous Chapter, for approximating the solution of the fractional advection equation.

Chapter 9

Time-Fractional Geometric Brownian Motion

9.1 Introduction

Many processes are geometrically scaled, with the process dynamics scaling with current values. This type of dynamics has been applied in numerous fields, including, as an example, the modelling of financial assets where returns are taken proportional to the current asset values. A particular stochastic process with geometric scaling is geometric Brownian motion. This Markovian process underlies many models, including the Black-Scholes option pricing framework [31].

Brownian motion can be derived as the diffusion limit of a CTRW with a Markovian exponential waiting time density. The CTRW is a stochastic process that tracks the position of a particle in time. The particle waits at some position for a random time, governed by the waiting time probability density function, before jumping a distance, governed by a jump length density, to a new location. CTRWs have been used as models in finance [123, 77, 132, 103, 100, 110], physics [111, 80, 67, 106], and biology [150, 68]. By taking a power-law tailed waiting time density, where the first moment diverges, the diffusion limit of the CTRW provides a stochastic model for anomalous diffusion where the mean squared displacement scales as a sub-linear power-law in time [106]. This stochastic model for subdiffusion is often referred to as fractional diffusion. Fractional diffusion is distinct from fractional Brownian motion. The latter is a Brownian motion with correlated noise [98].

In direct applications of CTRWs to finance it has generally been considered that the random walk involves the logarithm of the price of a financial issue. The logarithm of the price at a given time can be represented as a sum of log-returns at different trade times and the waiting time density governs the waiting time between trades [132, 103]. In this interpretation a waiting time density with a power-law decay, $\sim t^{-1-\alpha}$, with $0 < \alpha < 1$, results in sub-linear power-law scaling, $\sim t^{\alpha}$, of the mean squared logarithm of the price. In our analysis below, for a CTRW leading to fractional geometric Brownian motion, we find that a waiting time density with this power-law decay results in sub-linear power-law scaling, $\sim t^{\alpha}$, of the logarithm of the price.

In previous work, the effects of a force have been incorporated into CTRWs using biased jump length densities [28, 142, 61, 11]. The force can be introduced in this way through the assumption that the equilibrium distribution of particles subject to a conservative force is the Boltzmann distribution. The jump bias can also be defined as a difference between Boltzmann factors and, to lowest order in the lattice spacing, this is proportional to the force [61]. The diffusion limit of CTRWs with biased jump length densities and power-law waiting times leads to fractional Fokker-Planck equations [28, 142, 61, 11].

Typically, CTRWs are considered where the length of the jumps are independent of the position of the particle. In the analysis here we consider a multiplicative jump length density in which the jump length is proportional to the particle's current position. This naturally leads to the consideration of the process on a geometric lattice, where the position of neighbouring lattice sites differs by some multiplicative constant. The lattice effect is not prominent in the generalised master equation describing the CTRW, but care needs to be taken, with the implementation of the diffusion limit and the formulation of the bias consistent with a steady state Boltzmann distribution, to obtain the reduction to a Fokker-Planck equation. The diffusion limit of the CTRW with a power-law waiting time density and biased nearest neighbour steps on the geometric lattice leads to a time-fractional geometric

Fokker-Planck equation with spatially dependent diffusivity, and an additional advection term. If the bias is consistent with the force from a logarithmic potential, the fractional geometric Fokker-Planck equation reduces to the governing equation of a geometric Brownian motion as the anomalous exponent is taken to one. Hence the diffusion limit of the CTRW with a power-law waiting time density, and a multiplicative jump length density biased by a logarithmic potential, defines a fractional geometric Brownian motion, also referred to as subdiffusive geometric Brownian motion [94].

Formally, Magdziarz [94] introduced subdiffusive geometric Brownian motion, $Z_\alpha(t)$, as geometric Brownian motion, $Z(t)$, subordinated by an inverse α-stable subordinator $S_\alpha(t)$, i.e., $Z_\alpha(t) = Z(S_\alpha(t))$. In earlier work it had been shown that subdiffusive Brownian motion, ie., a Brownian motion in which the mean square displacement grows as a sub-linear power-law in time, can be obtained from Brownian motion subordinated by an inverse α-stable subordinator [106]. The governing evolution equation for the probability density function of a Brownian motion, or a geometric Brownian motion, subordinated by an inverse α-stable subordinator can readily be obtained using Laplace transform methods.

In geometric Brownian Motion the mean squared displacement grows as an exponential function in time, and in subdiffusive Brownian motion the mean squared displacement grows as a Mittag-Leffler function with time. For geometric processes, however, it is more insightful to consider the behaviour of the expectation of the logarithm of the position of the particle rather then the mean squared displacement. In finance this would be considered to be the expected logarithmic return. In the case of a geometric Brownian motion the expected logarithmic return grows linearly in time. Here we find that the expected logarithmic return of the geometric fractional diffusion grows as a sub-linear power-law in time, analogous to the mean square displacement scaling in anomalous sub-diffusion.

In section 9.2 we obtain the generalized master equation for a CTRW on a geometric lattice with nearest neighbour biased jumps. In the special case of Mittag-Leffler distributed waiting times, a waiting time density with a power-law tail, the generalised master equation becomes a fractional order differential equation. In section 9.3 we consider the diffusion limit of this generalized master equation. This limit involves the lattice spacing going to zero, and a characteristic waiting time going to zero, but at different rates to avoid singularities. The bias probabilities are dependent on the lattice spacing parameter so that the diffusion limit is dependent on the formulation of these probabilities. We consider a formulation that is consistent with a Boltzmann distribution for the steady state. The diffusion limit of the master equation for the CTRW on the geometric lattice with biased nearest neighbour jumps, and Mittag-Leffler distributed waiting times result is a fractional geometric Fokker-Planck equation. In section 9.4 we show that if the bias is consistent with a force from a logarithmic potential the diffusion limit provides a fractional generalisation of geometric Brownian motion previously identified through subordination methods as subdiffusive geometric Brownian motion [94]. In section 9.5 we calculate the moments, and the logarithmic moments, of this fractional geometric Brownian motion. We find that the logarithmic moments scale as a power-law in time. Finally in section 9.6 we provide a summary and discussion, and we have included an appendix showing how the fractional geometric Fokker-Planck equation can be obtained from the fractional Fokker-Planck equation with an appropriate change of variables and the introduction of an effective potential.

9.2 Generalized Master Equations for CTRWs on a Geometric Lattice

We consider a CTRW on a lattice x_i with a separable transition density,

$$\Psi(x_i, t|x_j, t') = \lambda(x_i, t, x_j)\psi(t - t'), \tag{9.1}$$

representing the probability density for a particle located at x_j at time t' to transition to x_i at time t. Here, $\lambda(x_i, t, x_j)$ is the probability density for a particle to jump from x_j to x_i at time t and $\psi(t, t')$ is the probability density for waiting from time t' to time t before jumping. The time dependence in the jump length density enables the inclusion of a time dependent bias, or time dependent force. The jump length density and the waiting time density are normalised as follows;

$$\sum_i \lambda(x_i, t, x_j) = 1, \tag{9.2}$$

and

$$\int_0^\infty \psi(t)dt = 1. \tag{9.3}$$

The generalised master equation for this CTRW, with a delta function initial condition, is given by [7]

$$\frac{\partial}{\partial t}\rho(x_i, t) = \sum_j \lambda(x_i, t, x_j) \int_0^t K(t - t')\rho(x_j, t')dt' - \int_0^t K(t - t')\rho(x_i, t')dt', \tag{9.4}$$

where $\rho(x_i, t)$ is the probability of finding the particle at site x_i at time t. In this equation $K(t)$ is a memory kernel defined by

$$K(t) = \mathcal{L}_s^{-1}\left\{\frac{\mathcal{L}_t\{\psi(t)\}}{\mathcal{L}_t\{\phi(t)\}}\right\}, \tag{9.5}$$

where $\mathcal{L}_t$ represents a Laplace transform from t to s, and $\mathcal{L}_s^{-1}$ an inverse Laplace transform from s to t, and $\phi(t)$ is the survival function defined as

$$\phi(t) = \int_t^\infty \psi(t')dt'. \tag{9.6}$$

If we consider a geometric lattice of points, $x_i \in (0, \infty)$, such that, $x_i = U^i$ for some parameter $U > 1$ then the master equation governs the evolution of the probability density function for a CTRW on a geometric lattice.

9.2.1 Multiplicative Jump Length Density

A CTRW with a multiplicative jump length density can now be constructed by considering nearest neighbour steps on the geometric lattice. The jump length density in this case is proportional to the current position of the particle. On this geometric lattice if a particle is at position x_i the nearest neighbour to the right is $x_{i+1} = Ux_i$ and the nearest neighbour to the left is $x_{i-1} = \frac{x_i}{U}$. The biased nearest neighbour jump probability density, to jump from site x_j to x_i, on this lattice is then,

$$\begin{aligned} \lambda(x_i, t, x_j) &= p_r(x_j, t)\delta[i - j - 1] + p_l(x_j, t)\delta[i - j + 1] \\ &= p_r(x_j, t)\delta[x_i - Ux_j] + p_l(x_j, t)\delta\left[x_i - \frac{x_j}{U}\right], \end{aligned} \tag{9.7}$$

where $\delta[z]$ is a Kronecker delta function, such that $\delta[z] = 1$ for $z = 0$ and $\delta[z] = 0$, for $z \neq 0$. The bias is introduced through $p_r(x_j, t)$, the probability of a jump to the right from the lattice site x_j at time t, and $p_l(x_j, t)$, the probability of a jump to the left from lattice site x_j at time t. The bias probabilities are normalised through

$$p_l(x_j, t) + p_r(x_j, t) = 1. \tag{9.8}$$

Note that the lattice spacing is not a fixed constant on the geometric lattice. In the analysis below we consider a diffusion limit with the lattice spacing approaching zero. In the geometric lattice the lattice spacing is zero if $U = 1$. It is convenient to define $U = 1 + u$, in which case the diffusion limit on the geometric lattice requires the limit $u \to 0$. We we can rewrite $\lambda(x_i, t, x_j)$ as,

$$\lambda(x_i, t, x_j) = p_r(x_j, t)\delta[x_i - (1 + u)x_j] + p_l(x_j, t)\delta\left[x_i - (1 + u)^{-1}x_j\right]. \tag{9.9}$$

The generalised master equation for a CTRW with biased nearest neighbour jumps on a geometric lattice can be found by substituting Eq. (9.9) into Eq. (9.4). The

result is

$$\begin{aligned}\frac{\partial}{\partial t}\rho(x_i,t) &= \int_0^t K(t-t')p_r(\frac{x_i}{1+u},t)\rho(\frac{x_i}{1+u},t')dt' \\ &+ \int_0^t K(t-t')p_\ell((1+u)x_i,t)\rho((1+u)x_i,t')dt' \\ &- \int_0^t K(t-t')\rho(x_i,t')dt'. \end{aligned} \tag{9.10}$$

9.2.2 Power-Law Waiting Time Density

We now consider the special case of a Mittag-Leffler distributed waiting time, with time scale τ and scaling exponent α,

$$\psi(t) = t^{1+\alpha}\tau E_{\alpha,\alpha}\left(-\tau t^\alpha\right), \tag{9.11}$$

with $0 < \alpha < 1$. The corresponding survival function is given by,

$$\phi(t) = E_{\alpha,1}\left(-\tau t^\alpha\right), \tag{9.12}$$

and the memory kernel can be written as,

$$K(t) = \mathcal{L}_s^{-1}\left\{\tau^{-\alpha}s^{1-\alpha}\right\}. \tag{9.13}$$

Evaluating the inverse Laplace transform leads to the introduction of fraction derivatives. Explicitly,

$$\int_0^t K(t-t')\rho(x_i,t')dt' = \tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\rho(x_i,t)\right). \tag{9.14}$$

The generalised master equation for biased nearest neighbour jumps, and Mittag-Leffler distributed waiting times on the geometric lattice, Eq. (9.10), can now be

written as a fractional order differential equation,

$$\begin{aligned}\frac{\partial}{\partial t}\rho(x_i,t) =& p_r\left((1+u)^{-1}x_i,t\right)\tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\rho\left((1+u)^{-1}x_i,t\right)\right)\\ &+ p_l((1+u)x_i,t)\tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\rho((1+u)x_i,t)\right) - \tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(\rho(x_i,t)\right).\end{aligned} \tag{9.15}$$

9.3 Diffusion Limit Fractional Fokker-Planck Equations

In this section we consider the diffusion limit of the master equation, Eq. (9.15). In this limit we are seeking the evolution equation for a space and time continuous probability density function. The diffusion limit involves taking the characteristic time $\tau \to 0$, and the lattice spacing parameter $u \to 0$, at controlled rates to avoid singularities. The bias probabilities are dependent on the lattice spacing parameter and thus they need to be treated in a consistent way.

We begin by embedding the discrete space probability density function $\rho(x_i,t)$, into a space continuous function, $\rho_u(x,t)$, that is parameterised by u. The function $\rho_u(x,t)$ is defined to be equal to $\rho(x_i,t)$, at all points $x = x_i$. The space continuous function $\rho_u(x,t)$ is not a probability density. However we can defined a probability density function $S(x,t)$ from $\rho_u(x,t)$ by considering the normalisation of $\rho(x_i,t)$. Starting with the normalisation

$$\sum_{i=-\infty}^{\infty}\rho(x_i,t) = 1, \tag{9.16}$$

and introducing a space dependent lattice spacing $\Delta x_i = ux_i$, we can write

$$\sum_{i=-\infty}^{\infty}\frac{\rho_u(x_i,t)}{ux_i}\Delta x_i = 1, \tag{9.17}$$

so that provided the limits exist,

$$\lim_{\Delta x_i\to 0}\sum_{i=-\infty}^{\infty}\left(\lim_{u\to 0}\frac{\rho_u(x_i,t)}{ux_i}\right)\Delta x_i = 1. \tag{9.18}$$

We now define

$$f_u(x,t) = \frac{\rho_u(x,t)}{ux}, \tag{9.19}$$

and then Eq. (9.18) expresses the normalisation

$$\int_0^\infty f(x,t)\,dx = 1, \tag{9.20}$$

where

$$f(x,t) = \lim_{u\to 0} f_u(x,t). \tag{9.21}$$

Rewriting the master equation, Eq. (9.15) in terms of the probability density function f_u gives,

$$\begin{aligned}\frac{\partial}{\partial t}f_u(x_i,t) &= p_r\left((1+u)^{-1}x_i,t\right)\tau^{-\alpha}(1+u)^{-1}\,{}_0\mathcal{D}_t^{1-\alpha}\left(f_u\left((1+u)^{-1}x_i,t\right)\right)\\ &+ p_l((1+u)x_i,t)(1+u)\tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(f_u((1+u)x_i,t)\right) - \tau^{-\alpha}\,{}_0\mathcal{D}_t^{1-\alpha}\left(f_u(x_i,t)\right).\end{aligned} \tag{9.22}$$

A Fokker-Planck equation will be found as the diffusion limit of this equation as $u \to 0$, and $\tau \to 0$. This limit will depend on the form taken for the bias jump probabilities. We consider definite forms for $p_r(x,t)$ and $p_\ell(x,t)$ in the next section.

9.3.1 Diffusion Limit

It is convenient to express the difference between the right and left jump probabilities in terms of a bias function, and so we define,

$$B_u(x_i,t) = p_r(x_i,t) - p_l(x_i,t). \tag{9.23}$$

This bias function has an implicit dependence on the scale parameter u. We may rewrite Eq. (9.22) in terms of the bias function,

$$\begin{aligned}\frac{\partial}{\partial t}f_u(x_i,t) &= \frac{1}{2}\tau^{-\alpha}(1+u)^{-1}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f_u\left((1+u)^{-1}x_i,t\right)\right)\\ &+\frac{1}{2}(1+u)\tau^{-\alpha}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f_u((1+u)x_i,t)\right)-\tau^{-\alpha}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f_u(x_i,t)\right)\\ &+B_u((1+u)^{-1}x_i,t)\tau^{-\alpha}(1+u)^{-1}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f_u\left((1+u)^{-1}x_i,t\right)\right)\\ &-B_u((1+u)x_i,t)(1+u)\tau^{-\alpha}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f_u((1+u)x_i,t)\right).\end{aligned} \tag{9.24}$$

Taking $x_i = x$, performing a Taylor expansion around $u = 0$, we can write,

$$\begin{aligned}\frac{\partial}{\partial t}f(x,t) &= \frac{u^2}{2\tau^\alpha}\frac{\partial}{\partial x}\Big(x(1+2B_0(x,t)-4b_0(x,t))\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)\\ &+x^2\frac{\partial}{\partial x}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)\Big)-\frac{2u}{\tau^\alpha}\frac{\partial}{\partial x}\left(xB_0(x,t)\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)\right)+O(u^3),\end{aligned} \tag{9.25}$$

where

$$B_0(x,t) = \lim_{u\to 0} B_u(x,t) \tag{9.26}$$

and

$$b_0(x,t) = \lim_{u\to 0}\frac{\partial}{\partial u}B_u(x,t). \tag{9.27}$$

The diffusion limit is found by taking the limit $u \to 0$ and $\tau \to 0$, such that,

$$\lim_{u,\tau\to 0}\frac{u^2}{2\tau^\alpha} = D_\alpha. \tag{9.28}$$

In order for the diffusion limit of Eq. (9.25) to exist we require $B_0(x,t) = 0$, and taking the limit gives,

$$\frac{\partial}{\partial t}f(x,t) = D_\alpha\frac{\partial}{\partial x}\left(x(1-4b_0(x,t))\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)+x^2\frac{\partial}{\partial x}\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)\right). \tag{9.29}$$

If the bias function does not depend on time then we can re-write Eq. (9.29) as follows:

$$ {}_0\mathcal{D}_t^{\alpha} f(x,t) = D_{\alpha} \frac{\partial}{\partial x} \left(x(1 - 4b_0(x)) \left(f(x,t) \right) + x^2 \frac{\partial}{\partial x} \left(f(x,t) \right) \right). \tag{9.30} $$

The asymptotic long time steady state for a conservative system acted on by a stationary potential $V(x)$ is the Boltzmann distribution,

$$ \lim_{t \to \infty} f(x,t) = \bar{f}(x) \propto e^{-\beta V(x)}, \tag{9.31} $$

where β is a parameter. If we substitute this steady state solution into Eq.(9.30), and consider the long time limit where the left hand side of the equation is zero, then we obtain an explicit expression relating the potential to the bias, viz;

$$ V(x) = \int_a^x \frac{1 - 4b_0(z)}{\beta z} dz. \tag{9.32} $$

where a is an arbitrary constant. From the identification

$$ F(x,t) = -\frac{\partial V(x,t)}{\partial x}. \tag{9.33} $$

we have the corresponding relation between the force $F(x)$ and the bias, viz;

$$ F(x) = \frac{4b_0(x) - 1}{\beta x}. \tag{9.34} $$

Thus in the case were the force does not depend on time we can write Eq. (9.29) as

$$ \frac{\partial f(x,t)}{\partial t} = D_{\alpha} \frac{\partial}{\partial x} \left(x^2 \frac{\partial}{\partial x} \, {}_0\mathcal{D}_t^{1-\alpha} f(x,t) - \beta x^2 F(x) \, {}_0\mathcal{D}_t^{1-\alpha} f(x,t) \right) \tag{9.35} $$

If the bias function depends explicitly on time we can generalize the expression in Eq. (9.34) to define

$$ b_0(x,t) = \frac{1}{4} \left(1 + \beta x F(x,t) \right) \tag{9.36} $$

and then Eq.(9.29) becomes

$$\frac{\partial f(x,t)}{\partial t} = D_\alpha \frac{\partial}{\partial x}\left(x^2 \frac{\partial}{\partial x}\, {}_0\mathcal{D}_t^{1-\alpha} f(x,t) - \beta x^2 F(x,t)\, {}_0\mathcal{D}_t^{1-\alpha} f(x,t)\right). \tag{9.37}$$

This equation is the fractional geometric Fokker-Planck equation for a particle subject to a space and time dependent force. In contrast to the standard fractional Fokker-Planck equation with space- and time- dependent forcing [61] we see a spatially dependent diffusivity and an additional spatial dependence on a force.

9.4 Fractional Geometric Brownian Motion

In this section we show that a fractional geometric Brownian motion can be defined from the fractional geometric Fokker-Planck equation with a force

$$F(x) = -\frac{v}{\beta x}. \tag{9.38}$$

This force can be derived from a logarithmic potential

$$V(x) = \frac{v}{\beta} \ln x, \tag{9.39}$$

where v is an arbitrary parameter and $v = 0$ corresponds to the case with no force. Substituting the force, defined by Eq. (9.38), into Eq. (9.37) we arrive at

$$\frac{\partial}{\partial t} f(x,t) = \frac{\partial}{\partial x}\left(x^2 \frac{\partial}{\partial x} D_\alpha\, {}_0\mathcal{D}_t^{1-\alpha} f(x,t)\right) + \frac{\partial}{\partial x}\left(v x D_\alpha\, {}_0\mathcal{D}_t^{1-\alpha} f(x,t)\right). \tag{9.40}$$

If we set $\alpha = 1$, $v = 2 - \frac{\mu}{D_1}$ and $D_1 = \frac{\sigma^2}{2}$ then Eq.(9.40) reduces to

$$\frac{\partial}{\partial t} f = \frac{x^2\sigma^2}{2}\frac{\partial^2 f}{\partial x^2} + (\sigma^2 - \mu) f + (2\sigma^2 - \mu) x \frac{\partial f}{\partial x}, \tag{9.41}$$

which is the Fokker-Planck equation for geometric Brownian motion. With the initial condition $\omega(x,0) = \delta(x-1)$, this has the solution,

$$f(x,t) = \frac{1}{\sqrt{2\pi t}\sigma x} \exp\left(-\frac{(\ln(x) - (\mu - \frac{\sigma^2}{2})t)^2}{2\sigma^2 t}\right). \tag{9.42}$$

Geometric Brownian motion has been widely used in financial mathematics as the stochastic process for modelling the price of an asset X_t assuming that percentage changes are independent and identically distributed. Geometric Brownian motion satisfies the stochastic differential equation

$$dX_t = \mu X_t + \sigma X_t dW_t, \tag{9.43}$$

where W_t is a Brownian motion. In financial applications, μ is the percentage drift and σ is the percentage volatility. We could equivalently write the stochastic differential equation as

$$dX_t = (2-v)D_1 X_t dt + \sqrt{2D_1} X_t dW_t, \tag{9.44}$$

which relates it back to the force defined in Eq. (9.38).

The generalized Fokker-Planck equation, Eq. (9.40), is the Fokker-Planck equation for a fractional geometric Brownian motion. The solution of Eq. (9.40), can be simply related to the solution of Eq. (9.41) using time subordination [94]. Explicitly, it is easy to verify using Laplace transform methods (see, e.g., the appendices in [94, 84]), that the solution of Eq. (9.40) is given by

$$f(x,t) = \int_0^\infty f^\star(x,\tau)\phi(\tau,t)\,dt \tag{9.45}$$

where $f^\star(x,t)$ is the solution of Eq. (9.41) and $\phi(\tau,t)$ has the Laplace transform

$$\hat{\phi}(\tau,s) = \int_0^\infty \phi(\tau,t)s^{-st}\,dt = s^{\alpha-1}e^{-\tau s^\alpha}. \tag{9.46}$$

9.5 Moments

In this section we consider the moments and logarithmic moments of the fractional geometric Brownian motion. We begin by considering expressions for the moments of the fractional geometric Fokker-Planck equation, Eq. (9.37). The n^{th} moment is defined as,

$$\langle x^n(t)\rangle = \int_0^\infty x^n f(x,t)dx. \tag{9.47}$$

To check that the equation is conservative we begin by considering the zeroth moment. Integrating both sides of Eq. (9.37) with respect to x, and integrating we find,

$$\frac{d\langle x^0(t)\rangle}{dt} = 0, \tag{9.48}$$

provided that $\int_0^\infty S(x,t)dx$ exists. Hence the zeroth moment is conserved as expected. The first moment, or mean, is found by first multiplying both sides of Eq. (9.37) by x and then integrating over x, this gives,

$$\frac{d\langle x(t)\rangle}{dt} = 2D_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle x(t)\rangle\right) + \beta D_\alpha \int_0^\infty x^2 F(x,t)\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)dx. \tag{9.49}$$

In general the integro-differential equation that governs the evolution of the n^{th} moment is,

$$\frac{d\langle x^n(t)\rangle}{dt} = n(n+1)D_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle x^n(t)\rangle\right) + n\beta D_\alpha \int_0^\infty x^{n+1} F(x,t)\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right)dx. \tag{9.50}$$

This fractional integro-differential equation simplifies for fractional geometric Brownian motion.

We have also considered the log-moments of the fractional geometric Fokker-Planck equation, Eq.(9.37). The n^{th} log-moment is defined as,

$$\langle(\ln(x(t)))^n\rangle = \int_0^\infty (\ln(x(t)))^n f(x,t)dx. \tag{9.51}$$

If x represents the price of an asset then the first log-moment is the expected logarithmic return. Similar to the moment calculations we multiply Eq. (9.37) by $(\ln(x))^n$ and integrate with respect to x, this leads to the evolution of the n^{th} log-moment to be governed by,

$$\begin{aligned}\frac{d\langle(\ln(x(t)))^n\rangle}{dt} =& n(n-1)D_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle(\ln(x(t)))^{n-2}\rangle\right) + nD_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle(\ln(x(t)))^{n-1}\rangle\right) \\ &+ n\beta D_\alpha \int_0^\infty (\ln(x))^{n-1} x F(x,t)\ {}_0\mathcal{D}_t^{1-\alpha}\left(f(x,t)\right) dx.\end{aligned} \tag{9.52}$$

Again, this fractional integro-differential equation simplifies for fractional geometric Brownian motion.

9.5.1 Fractional Geometric Brownian Motion Moments

In section 9.4 we showed that the probability density function for a fractional geometric Brownian motion is governed by the fractional geometric Fokker-Planck equation with the force, Eq. (9.38), derived form a logarithmic potential. We now substitute the expression for the force, Eq. (9.38), into Eq. (9.50) to obtain the moments for the fractional geometric Brownian motion. This yields,

$$\frac{d\langle x^n(t)\rangle}{dt} = \left(n(n+1) - nv\right) D_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle x^n(t)\rangle\right). \tag{9.53}$$

With the given initial condition, the solution of Eq. (9.53) is a Mittag-Leffler function,

$$\langle x^n(t)\rangle = E_\alpha\left((n(n+1) - nv)D_\alpha t^\alpha\right). \tag{9.54}$$

From this it is easy to see that the mean will be,

$$\langle x(t)\rangle = E_\alpha\left((2-v)D_\alpha t^\alpha\right). \tag{9.55}$$

Next we can consider the log-moments. Using the force from the logarithmic potential, Eq. (9.52) becomes,

$$\begin{aligned}\frac{d\langle(\ln(x(t)))^n\rangle}{dt} &= n(n-1)D_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle(\ln(x(t)))^{n-2}\rangle\right)\\ &+ n(1-v)D_\alpha\ {}_0\mathcal{D}_t^{1-\alpha}\left(\langle(\ln(x(t)))^{n-1}\rangle\right)\end{aligned} \tag{9.56}$$

For $n = 1$ this simplifies to,

$$\frac{d\langle(\ln(x(t)))\rangle}{dt} = (1-v)\frac{D_\alpha}{\Gamma(\alpha)}t^{\alpha-1}, \tag{9.57}$$

where we have used the following property of a Riemann-Liouville fractional derivative,

$${}_0\mathcal{D}_t^{1-\alpha}\,(1) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}. \tag{9.58}$$

Using our initial conditions we can see that, $\langle(\ln(x(0)))\rangle = 0$, and so Eq. (9.57) has the solution,

$$\langle(\ln(x(t)))\rangle = \frac{(1-v)D_\alpha}{\Gamma(1+\alpha)}t^\alpha \tag{9.59}$$

Note that for geometric Brownian motion, $\alpha = 1$, the log moment scales linearly with time whereas for fractional geometric Brownian motion the log moment scales as a sub-linear power-law in time. This is analogous to the sub-linear power-law scaling of the mean square displacement in anomalous subdiffusion [106].

9.6 Summary

In this Chapter we have considered the CTRW on a geometric lattice, with biased jumps related to a force and, in the case of a power-law tailed waiting time density, the diffusion limit results in a fractional geometric Fokker-Planck equation. In carrying out the diffusion limit we considered the relation between the bias and a force derived from a potential. Our approach has been to consider the relationship that emerges by requiring the steady state solution, if it exists, to be the Boltzmann distribution.

We have further shown that if the force is obtained from a logarithmic potential then the corresponding geometric fractional Fokker-Planck equation governs the evolution of the probability density function for a fractional, or subdiffusive, geometric Brownian motion. We have obtained expressions for the moments, and the logarithmic moments, of the subdiffusive geometric Brownian motion. One of the signature properties of the subdiffusive geometric Brownian motion is that the log moment was shown to scale as a sublinear power-law in time.

Chapter 10

Anomalous Diffusion on an Arbitrarily Growing Domain

10.1 Introduction

A wide range of important physical phenomena involve transport in expanding, and contracting, domains. Fundamental examples include, the diffusion of proteins within growing cells, the interactions of cells in a growing organism, and diffusion in an expanding universe. The governing equations for reaction diffusion on growing domains and related studies of pattern formation have been considered in a series of publications, see for example, [36, 113, 37, 26, 153, 155, 140, 157]. Domain growth has been shown to be fundamentally important to the development of patterns [81].

In this Chapter we derive the equation for anomalous diffusion occurring on an arbitrarily growing domain. This follows the derivation in [23]. We start with the underlying stochastic process of a CTRW to derive master equations for subdiffusive transport in a growing domain. In our derivation we first consider a mapping between a given position x on the domain at time $t = 0$ and the position that it evolves to, y, on the growing domain at a later time t. With this mapping we then transform the CTRW from the coordinates on the growing domain to a non-growing fixed domain. An auxiliary master equation for the evolution of the density on the fixed domain is derived. The auxiliary master equation is constructed so that the value of the density at a given x and t equates to the probability density on the growing domain for y and t. The diffusion limit of the master equation is taken to produce a fractional diffusion equation on both the fixed and growing domains.

Our approach enables us to model subdiffusive transport of particles on arbitrarily growing domains, and the solution of the auxiliary master equation on the fixed domain could be used as the basis for numerical simulations of subdiffusive transport on growing domains. The equations we derive on the growing domain can be interpreted phenomenologically as a reaction sub-diffusion process with an additional advective term. In this context, the reaction represents the dilution of the concentration due to the growing domain. The remainder of this Chapter is organised as follows. In Section 10.2 we establish the mapping between the arbitrarily growing domain and the initial fixed domain. In Section 10.3 we derive the master equation on the initial domain and map it onto growing domain of interest.

10.2 Mapping

We wish to construct a mapping between a location on the initial fixed domain, $x \in [0, L_0]$, to the corresponding location at some later time t, on the growing domain $y \in [0, L(t)]$. To characterise how the domain is changing in time we begin by partitioning the domain $[0, L_0]$ into m cells of width $\delta x = \frac{1}{m}$. The ith partition begins at position $x_i = i\delta x$. As the domain grows, the width of the partitions, now denoted by $\delta y_i(t)$ will have grown with the domain and formed a partition of $[0, L(t)]$. Note that whilst the initial cell widths were constant this is no longer the case in the growing domain, i.e. δy_i is a function of both the initial position x_i and time. The mapping is defined through a growth function, $\mu(x_i, t)$, via,

$$\frac{1}{\delta y_i}\frac{d\delta y_i}{dt} = \mu(x_i, t). \tag{10.1}$$

Explicitly it can be shown that the mapping $g(x, t)$ from a position in the fixed domain, x, to a corresponding position on the growing domain, y, is given by,

$$y = \lim_{n\to\infty}\sum_{i=1}^{n}\delta y_i = \int_0^x \exp\left(\int_0^t \mu(z, s)ds\right)dz = g(x, t). \tag{10.2}$$

This is illustrated schematically in Figure 10.1. Note that, $g(0,t) = 0$ and the initial condition, $y = g(x,0) = x$ for all $x \in [0, L_0]$, places a physical restriction on the mapping between y and x. For future notational convenience we will denote the spatial derivative of $g(x,t)$ as $\nu^*(x,t)$, so that,

$$\nu^*(x,t) = \frac{\partial g(x,t)}{\partial x} = e^{\int_0^t \mu(x,s)ds}, \tag{10.3}$$

and the time derivative as,

$$\eta^*(x,t) = \frac{\partial g(x,t)}{\partial t} = \int_0^x \mu(z,t) e^{\int_0^t \mu(z,s)ds} dz. \tag{10.4}$$

As the mapping is invertible, so that $x = g^{-1}(y,t)$, these can be expressed on the growing domain, giving,

$$\nu(y,t) = \nu^*(g^{-1}(y,t),t), \tag{10.5}$$

and

$$\eta(y,t) = \eta^*(g^{-1}(y,t),t). \tag{10.6}$$

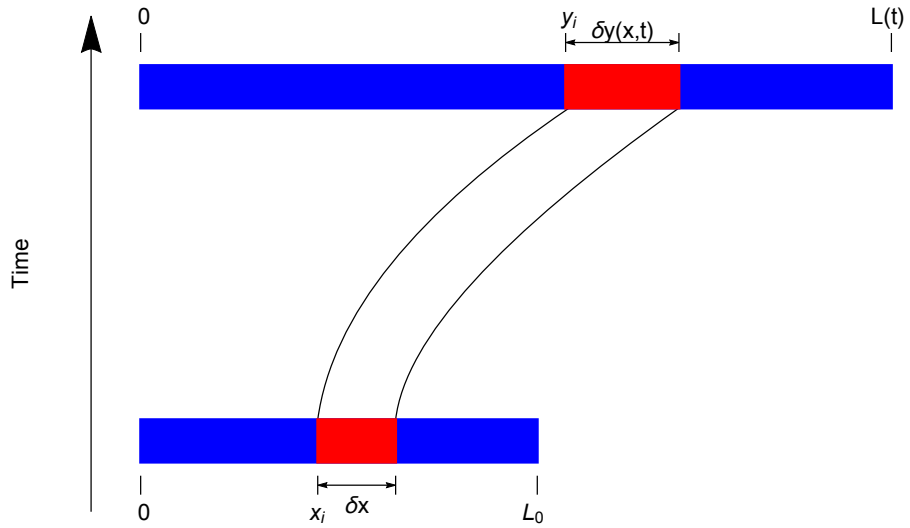

Figure 10.1: Schematic representation of the growth of the domain and the mapping of an interval in the initial domain to a corresponding interval at some later time t.

It should also be noted that if we consider the growth of a small interval in the initial domain $(x, x+\delta x)$, then the width of the interval at some later time, in the limit of small δx can be written as,

$$\delta y(x,t) = e^{\int_0^t \mu(x,s)ds}\delta x. \tag{10.7}$$

10.3 Master Equation

We now consider a CTRW on a growing domain, such that a particle will jump to a location, wait for some time, and then jump to a new location. We will assume that the waiting time and jump length densities are independent. The waiting time probability density for a particle that arrived at a location at time t' to jump at time t will be denoted by $\psi(t-t')$, where $t-t'$ is the amount of time that the particle waited. The jump length density for a particle that is at a location z' to jump to location z at time t is denoted by $\lambda(z|z',t)$. In the following we consider a CTRW on the growing domain $z=y$ and an auxiliary CTRW on the fixed domain $z=x$. In taking the diffusion limit we will restrict ourselves to fixed length jumps on the growing domain, Δy, where the particle may jump either left or right. The corresponding jumps in the auxiliary CTRW on the initial fixed domain will therefore have lengths that change in both time and space as the domain grows.

For a particle undergoing a CTRW on the growing domain, we let $\rho(y,t)\delta y(x,t)$ denote the probability of finding the particle in the region $(y, y+\delta y(x,t))$, in the time $(t, t+\delta t)$ for a small $\delta y(x,t)$. Thus $\rho(y,t)$ is the probability density of finding the particle, which we can express as follows,

$$\rho(g(x,t),t)\delta y(x,t) = \int_0^t \Phi(t-t')q(g(x,t'),t')\delta y(x,t')dt', \tag{10.8}$$

where $\Phi(t-t')$ is the survival function associated with the waiting time density $\psi(t-t')$. The inbound flux, $q(g(x,t),t)$, is defined such that the probability of the particle entering the region $(y, y+\delta y(x,t))$ in the time $(t, t+\delta t)$, given $y=g(x,t)$,

is $q(g(x,t),t)\delta y(x,t)\delta t$. This equation states that for a particle to be in the region, it must have previously arrived in the region and not jumped away.

Equation (10.8) can be simplified by using Eq. (10.7),

$$\rho(g(x,t),t)e^{\int_0^t \mu(x,s)ds} = \int_0^t \Phi(t-t')q(g(x,t'),t')e^{\int_0^{t'} \mu(x,s)ds}dt'. \tag{10.9}$$

To transform the evolution equation to a master equation it is necessary to replace the explicit dependence on $q(g(x,t),t)$ with a dependence on $\rho(g(x,t,),t)$. The growth of the domain requires us to utilise non-standard techniques to achieve this. As the region is moving and growing this is most easily expressed by mapping the required functions back to the fixed x domain. The formulation of the CTRW on the fixed domain will be referred to as an auxiliary CTRW.

To formulate the auxiliary CTRW on the fixed domain, we relate the associated densities to densities on the growing domain, such that,

$$\rho(y,t) = \rho(g(x,t),t) = \rho^*(x,t), \qquad q(g(x,t),t) = q^*(x,t). \tag{10.10}$$

Here we use a star to denote a function associated with the auxiliary process on the fixed domain. Hence we can write the auxiliary form of Eq. (10.9) as,

$$\rho^*(x,t)e^{\int_0^t \mu(x,s)ds} = \int_0^t \Phi(t-t')q^*(x,t')e^{\int_0^{t'} \mu(x,s)ds}dt'. \tag{10.11}$$

Note that this left hand side, $\rho^*(x,t)e^{\int_0^t \mu(x,s)ds}$, is a conserved probability density. Differentiating Eq. (10.11) with respect to time and simplifying, we arrive at an evolution equation for the probability density,

$$\frac{\partial \rho^*(x,t)}{\partial t} = q^*(x,t) - \int_0^t \psi(t-t')e^{-\int_{t'}^t \mu(x,s)ds}q^*(x,t')dt' - \mu(x,t)\rho^*(x,t). \tag{10.12}$$

In this equation the second term on the right hand side is the flux out of the neighbourhood around x in the time interval around t, while the third term is the

reduction in concentration of particles, around x around t, due to the growth of the domain. Explicitly we define the flux out as,

$$i^*(x,t) = \int_0^t \psi(t-t')q^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt'. \tag{10.13}$$

In this equation the incoming flux, $q^*(x,t)$, can itself be expressed in terms of the flux out resulting in the relation,

$$q^*(x,t) = \int_0^{L(0)} \lambda(x|x',t)i^*(x',t)dx', \tag{10.14}$$

where $\lambda(x|x',t)$ is the jump probability density, where a particle at x' jumps to x, at time t.

Using Eq. (10.14), noting the semi-group property of the exponential function, we can rewrite Eq. (10.12) and using Laplace transform methods, we can express the evolution equation for the auxiliary CTRW as the auxiliary master equation,

$$\begin{aligned}\frac{\partial \rho^*(x,t)}{\partial t} = &\int_0^{L(0)} \lambda(x|x',t) \int_0^t K(t-t')\rho^*(x',t')e^{-\int_{t'}^t \mu(x',s)ds}dt'dx' \\ &- \int_0^t K(t-t')\rho^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt' - \mu(x,t)\rho^*(x,t).\end{aligned} \tag{10.15}$$

In this equation, the memory kernel, $K(t)$, is defined by,

$$\mathcal{L}_t\{K(t)\} = \frac{\mathcal{L}_t\{\psi(t)\}}{\mathcal{L}_t\{\Phi(t)\}}, \tag{10.16}$$

where $\mathcal{L}_t$ denotes a Laplace transform with respect to time.

The master equation, Eq. (10.15), has been derived for arbitrary waiting time and jump densities. To obtain a diffusion limit of the master equation we will require specific forms for these densities. We wish to consider the case of a fixed jump length on the growing domain, where the particle will jump either right or left with equal probability. In this case the jump length for the auxiliary master

equation will change with both space and time. The jump probability density can therefore be written as,

$$\lambda(x|x',t) = \frac{1}{2}\left(\delta(x - x' - \epsilon^+) + \delta(x - x' + \epsilon^-)\right), \tag{10.17}$$

where $\delta(x)$ is the Dirac delta function, and ϵ^+ and ϵ^- are time and space dependent. To relate the ϵ's to the fixed jump length, Δy, we note that from Eq. (10.2) we have,

$$\Delta y = \int_{x-\epsilon^+}^{x} e^{\int_0^t \mu(z,s)ds} dz, \tag{10.18}$$

$$\Delta y = \int_{x}^{x+\epsilon^-} e^{\int_0^t \mu(z,s)ds} dz. \tag{10.19}$$

Using the relations from Eqs. (10.18) and (10.19), we perform a Taylor expansion of Eq. (10.15) with the jump distribution given by, Eq. (10.17) around $\Delta y = 0$ to arrive at,

$$\begin{aligned}\frac{\partial \rho^*(x,t)}{\partial t} = \frac{\Delta y^2 e^{-2\int_0^t \mu(x,s)ds}}{2} &\left(\left(\frac{\partial^2}{\partial x^2}\int_0^t K(t-t')\rho^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt'\right)\right. \\ &\left. - \left(\int_0^t \frac{\partial \mu(x,s)}{\partial x}ds\right)\left(\frac{\partial}{\partial x}\int_0^t K(t-t')\rho^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt'\right)\right) \\ &- \mu(x,t)\rho^*(x,t) + O(\Delta y^3).\end{aligned} \tag{10.20}$$

To consider subdiffusion on a growing domain we now take a heavy tailed Mittag-Leffler waiting time density, given by,

$$\psi(t) = \frac{t^{\alpha-1}}{\tau^\alpha} E_{\alpha,\alpha}\left(-\left(\frac{t}{\tau}\right)^\alpha\right), \tag{10.21}$$

with $0 < \alpha < 1$ and $\tau > 0$. The memory kernel of a Mittag-Leffler probability density can be calculated from the inverse Laplace transform of Eq. (10.16),

$$K(t) = \mathcal{L}_s^{-1}\left\{\frac{s^{1-\alpha}}{\tau^\alpha}\right\}. \tag{10.22}$$

Recall that the Riemann-Liouville fractional derivative of order $1-\alpha$ is defined as,

$$ {}_0\mathcal{D}_t^{1-\alpha}\left(f(t)\right) = \frac{1}{\Gamma(\alpha)}\frac{d}{dt}\int_0^t f(t')(t-t')^{\alpha-1}dt'. \tag{10.23} $$

As we are considering smooth real valued functions, the initial condition term in the Laplace transform of the Riemann-Liouville fractional derivative will be zero [89], so that,

$$ \mathcal{L}_t\left\{{}_0\mathcal{D}_t^{1-\alpha}\left(f(t)\right)\right\} = s^{1-\alpha}\mathcal{L}_t\left\{f(t)\right\}. \tag{10.24} $$

Using Mittag-Leffler distributed waiting times the auxiliary master equation on the fixed domain, Eq. (10.20), becomes,

$$ \begin{aligned} \frac{\partial\rho^*(x,t)}{\partial t} =& \frac{\Delta y^2 e^{-2\int_0^t \mu(x,s)ds}}{2\tau^\alpha}\left(\frac{\partial^2}{\partial x^2}\left(\frac{{}_0\mathcal{D}_t^{1-\alpha}\left(\rho^*(x,t)e^{\int_0^t\mu(x,s)ds}\right)}{e^{\int_0^t\mu(x,s)ds}}\right)\right. \\ &\left. -\left(\int_0^t\frac{\partial\mu(x,s)}{\partial x}ds\right)\frac{\partial}{\partial x}\left(\frac{{}_0\mathcal{D}_t^{1-\alpha}\left(\rho^*(x,t)e^{\int_0^t\mu(x,s)ds}\right)}{e^{\int_0^t\mu(x,s)ds}}\right)\right) \\ &-\mu(x,t)\rho^*(x,t)+\mathcal{O}(\Delta y^3). \end{aligned} \tag{10.25} $$

The fractional diffusion limit is one in which the length and time scales are taken to zero, such that,

$$ D_\alpha = \lim_{\Delta y,\tau\to 0}\frac{\Delta y^2}{2\tau^\alpha}, \tag{10.26} $$

exists. The fractional diffusion limit of Eq. (10.25) is,

$$ \begin{aligned} \frac{\partial\rho^*(x,t)}{\partial t} =& D_\alpha e^{-2\int_0^t\mu(x,s)ds}\left(\frac{\partial^2}{\partial x^2}\left(\frac{{}_0\mathcal{D}_t^{1-\alpha}\left(\rho^*(x,t)e^{\int_0^t\mu(x,s)ds}\right)}{e^{\int_0^t\mu(x,s)ds}}\right)\right. \\ &\left.-\left(\int_0^t\frac{\partial\mu(x,s)}{\partial x}ds\right)\frac{\partial}{\partial x}\left(\frac{{}_0\mathcal{D}_t^{1-\alpha}\left(\rho^*(x,t)e^{\int_0^t\mu(x,s)ds}\right)}{e^{\int_0^t\mu(x,s)ds}}\right)\right)-\mu(x,t)\rho^*(x,t). \end{aligned} \tag{10.27} $$

This is the auxiliary fractional diffusion equation defined on the fixed domain. Note that, apart from the advective type term, this is the same form as a fractional re-

action subdiffusion equation [7], with the additional feature of a space and time dependent diffusivity. In writing the equation in terms of the growing domain coordinates the diffusivity will be constant.

Boundary conditions may be implemented by considering different jump length densities near the boundary. Explicitly, a zero flux boundary will be implemented by taking,

$$\lambda(x|x',t) = \delta(x - x' + \epsilon^-), \tag{10.28}$$

for $x \in [L(0) - \epsilon^-, L(0)]$ and,

$$\lambda(x|x',t) = \delta(x - x' - \epsilon^+), \tag{10.29}$$

for $x \in [0, \epsilon^+]$. This jump density guarantees that there is no flux across the boundary, and in the diffusive limit the master equation at the boundary point will be consistent with the master equation in the bulk.

Using the jump length density for the left boundary, Eq. (10.29), and taking a Taylor expansion around $\Delta y = 0$, the master equation, Eq. (10.15), becomes,

$$\begin{aligned}\frac{\partial \rho^*(x,t)}{\partial t} &= \Delta y e^{-\int_0^t \mu(x,s)ds} \frac{\partial}{\partial x}\left(\int_0^t K(t-t')\rho^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt'\right) \\ &+ \frac{\Delta y^2 e^{-2\int_0^t \mu(x,s)ds}}{2}\left(\left(\frac{\partial^2}{\partial x^2}\int_0^t K(t-t')\rho^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt'\right)\right. \\ &\left. - \left(\int_0^t \frac{\partial \mu(x,s)}{\partial x}ds\right)\left(\frac{\partial}{\partial x}\int_0^t K(t-t')\rho^*(x,t')e^{-\int_{t'}^t \mu(x,s)ds}dt'\right)\right) \\ &- \mu(x,t)\rho^*(x,t) + O(\Delta y^3).\end{aligned} \tag{10.30}$$

for $x \in [0, \epsilon^+]$. The difference between this equation and the bulk result is the occurrence of a first order spatial derivative. With the Mittag-Leffler waiting time density in order for the diffusion limit, Eq. (10.26) to exist, we require the first order

spatial derivative term to be,

$$\frac{\partial}{\partial x}\left(\frac{{}_0\mathcal{D}_t^{1-\alpha}\left(\rho^*(x,t)e^{\int_0^t \mu(x,s)ds}\right)}{e^{\int_0^t \mu(x,s)ds}}\right)\Bigg|_{x=0} = 0, \tag{10.31}$$

only holding at the boundary point as $\Delta y \to 0$. This zero flux boundary condition is equivalent to the zero flux boundary derived for fractional reaction subdiffusion equations [10]. The derivation for the right hand side of the boundary results in an equivalent condition.

The fractional diffusion equation can be found by mapping the auxiliary equation, Eq. (10.27), to the growing domain. Using the mapping $y = g(x,t)$, with Eqs. (10.5) and (10.6), we perform a change of variables and find,

$$\begin{aligned}\frac{\partial \rho(y,t)}{\partial t} =& D_\alpha \frac{\partial^2}{\partial y^2}\left(\frac{1}{\nu(y,t)}\,{}_0^g\mathcal{C}_t^{1-\alpha}\left(\rho(y,t)\nu(y,t)\right)\right) - \eta(y,t)\frac{\partial \rho(y,t)}{\partial y} \\ &- \left(\frac{\partial \nu(y,t)}{\partial t}\right)\frac{1}{\nu(y,t)}\rho(y,t).\end{aligned} \tag{10.32}$$

Here we have defined a new comoving fractional derivative, ${}_0^g\mathcal{C}_t^{1-\alpha}$, which operates along the curve, $y = g(x,t)$, for a fixed x. Formally this is defined as,

$${}_0^g\mathcal{C}_t^{1-\alpha} f(y,t) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t f(g(g^{-1}(y,t),t'),t')(t-t')^{\alpha-1}dt'. \tag{10.33}$$

Informally, the history of the function is not integrated over a fixed value of y but rather along the trajectory of the point in the domain as it grows. As with the Riemann-Liouville fractional derivative, the co-moving fractional derivative becomes the identity operator in the limit as $\alpha \to 1$. We note that,

$${}_0^g\mathcal{C}_t^{1-\alpha}\left(\rho(y,t)\nu(y,t)\right) = {}_0\mathcal{D}_t^{1-\alpha}\left(\rho^*(x,t)\nu^*(x,t)\right). \tag{10.34}$$

The physical understanding of Eq. (10.32) is that the third term on the right hand side is a dilution factor due to the growing domain, the second term is an

advection factor due to the growing domain and the first term is a fractional diffusion term modified to take into account both the growth and dilution. The boundary condition, Eq. (10.31), on the growing domain is,

$$\frac{\partial}{\partial y}\left(\frac{{}_0^g\mathcal{C}_t^{1-\alpha}\left(\rho(y,t)\nu(y,t)\right)}{\nu(y,t)}\right)\Bigg|_{y=0,L(t)} = 0. \tag{10.35}$$

We note that when $\alpha \to 1$ this boundary condition is independent of the rate of the domain growth and is simplified to,

$$\frac{\partial \rho(y,t)}{\partial y}\Bigg|_{y=0,L(t)} = 0, \tag{10.36}$$

on the growing domain.

It should also be noted that,

$$\frac{d}{dt}\int_0^{L(t)} \rho(y,t)dy = 0. \tag{10.37}$$

This can be seen by integrating Eq. (10.32) over the growing domain and using the boundary conditions given by Eq. (10.35).

As a specific example, we consider a constant growth rate in which the mapping between the original and growing domain is defined by Eq. (10.2),

$$\mu(x,t) = r, \quad \text{and} \quad g(x,t) = xe^{rt}, \tag{10.38}$$

where $r \in \mathbb{R}$. Using this we can simplify the master equation on the growing domain, Eq. (10.32), and it becomes,

$$\frac{\partial \rho(y,t)}{\partial t} = D_\alpha \frac{\partial^2}{\partial y^2}\left(e^{-rt}\,{}_0^g\mathcal{C}_t^{1-\alpha}\left(\rho(y,t)e^{rt}\right)\right) - ry\frac{\partial \rho(y,t)}{\partial y} - r\rho(y,t), \tag{10.39}$$

with boundary conditions given by Eq. (10.35). This can be considered a simple model for diffusion of transmembrane proteins, such as potassium channels [99], that

are anomalously diffusing in the plasma membrane of a uniformly growing cell, for example during the G1 phase of growth of budding yeast [101]. In the case as $\alpha \to 1$, we recover the expected equation for diffusion on a uniformly growing domain, see Murray [113].

10.4 Summary

In this Chapter we have derived evolution equations that describe subdiffusive transport on a growing domain. Equation (10.27) describes the transport on a rescaled fixed domain whilst Eq. (10.32) describes the same process on the growing domain. The evolution equation on the growing domain required the definition of a new fractional order differential operator that follows the domain growth, Eq. (10.33). Our work provides the essential first step for modelling physical applications involving subdiffusion on growing domains. This model can be extended in numerous ways; including reactions through birth and death processes, including forces using biased CTRWs, and generalising to higher dimensions using a multidimensional growth function and multidimensional CTRWs.

Part III

Other Published Work on Discretisation Methods

Chapter 11

Piecewise Fractional ODE Method

11.1 Introduction

This Chapter follows the derivation in [16]. In the following we consider an initial value fractional-order ODE (frODE) of the form,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t) = f(x(t)),\ x(0) = x_0, \tag{11.1} $$

where ${}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}$ is a Caputo fractional derivative with $0 < \alpha < 1$ and $f(x(t))$ is potentially a nonlinear vector field. Extending the work of El-Sayed and others [49, 5, 69, 135, 47, 48, 51, 50] we provide a correct derivation of the difference equation approximation to Eq. (11.1) based on a piecewise approximation. This results in an increasing order difference equation which captures the memory effect of the frODE. This is achieved by a piecewise constant approximation of the vector field, resulting in a one parameter family of integrable frODEs that limit to the original frODE. The integrable frODEs have a closed form solution that can be discretised to provide a difference equation that approximates the solution of the original frODE. Furthermore, we show that this method may be implemented with an non-uniform time step. An example is presented that shows the difference equation correctly captures the dynamics of a specific frODE.

11.2 Fractional Derivatives

The properties of fractional derivatives were summarised in Chapter 1 but we have made further remarks here for convenience. There exist multiple types of fractional derivatives, here we will focus on frODEs involving Caputo derivatives. A Caputo fractional derivative is defined by [34],

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-t')^{-\alpha}\frac{dx(t')}{dt'}dt', \tag{11.2}$$

for $0 < \alpha < 1$. The Riemann-Liouiville fractional derivative is defined by,

$$ {}_{\mathrm{RL}}\mathcal{D}^{\alpha}_{0,t}x(t) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_0^t (t-t')^{-\alpha}x(t')dt', \tag{11.3}$$

for $0 < \alpha < 1$. We can transform a Caputo derivative to a Riemann-Liouville through the following relation [89];

$$ {}_{\mathrm{RL}}\mathcal{D}^{\alpha}_{0,t}(x(t) - x(0)) = {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t), \tag{11.4}$$

hence the two are equivalent when $x(0) = 0$.

Fractional derivatives can be easily expressed in Laplace space and we will make use of this form. The Laplace transform of the Caputo fractional derivative is,

$$ \mathcal{L}_t\{{}_C\mathcal{D}^{\alpha}_{0,t}x(t)\} = s^{\alpha}\mathcal{L}_t\{x(t)\} - s^{\alpha-1}x(0). \tag{11.5}$$

The Grünwald-Letnikov derivative is defined by,

$$ {}_{\mathrm{GL}}\mathcal{D}^{\alpha}_{0,t}x(t) = \lim_{\delta t\to 0}\frac{1}{\delta t^{\alpha}}\sum_{m=0}^{\infty}(-1)^m\begin{pmatrix}\alpha\\ m\end{pmatrix}x(t-m\delta t). \tag{11.6}$$

If $x(t) \in C^0$ and $0 < \alpha \leq 1$, then this is equivalent to the Riemann-Liouville derivative. Grünwald-Letnikov derivatives have long been used as a basis of methods for discretising Riemann-Liouville frODEs [121, 27].

11.3 Problems with First Order Approximations to frODEs

The approach taken by El-Sayed and others [49, 5, 69, 135, 47, 48, 51, 50] when applied to the fractional equation, Eq. (11.1), results in a discrete first order equation of the form,

$$x((n+1)\delta t) = x(n\delta t) + \frac{\delta t^\alpha}{\Gamma(1+\alpha)} f(x(n\delta t)). \tag{11.7}$$

We can use a simple convergence argument to demonstrate that this first order difference equation can not capture the dynamics of a fractional order differential equation.

11.3.1 Convergence

In this subSection we demonstrate that Eq. (11.7) does not converge to Eq. (11.1) as $\delta t \to 0$ such that $t = n\delta t$. Noting that the solution of Eq. (11.7) is a function that is only defined over a discrete set of points, we define a function of a continuous variable $y_\delta(t)$, such that at the points $t = n\delta t$ we have $y_\delta(t) = x(n\delta t)$. Away from these points the function $y_\delta(t)$ is defined as an interpolation whereby the resulting function is continuous and differentiable. We will assume that such a function will have a well behaved limit as $\delta t \to 0$ so that,

$$\lim_{\delta t \to 0} y_\delta(t) = y(t). \tag{11.8}$$

This limit must exist if Eq. (11.7) is to converge, furthermore if Eq. (11.7) did converge to Eq. (11.1) then $y(t)$ would be a solution of Eq. (11.1). We will now show that $y(t)$ is not a solution of Eq. (11.1).

From Eq. (11.7) we see that y_δ obeys the relation,

$$y_\delta((n+1)\delta t) = y_\delta(n\delta t) + \frac{\delta t^\alpha}{\Gamma(1+\alpha)} f(y_\delta(n\delta t)). \tag{11.9}$$

Letting $t = n\delta t$, we can rearrange Eq. (11.9) to give,

$$\Gamma(1+\alpha)\frac{(y_\delta(t+\delta t) - y_\delta(t))}{\delta t^\alpha} = f(y_\delta(t)). \tag{11.10}$$

Taking a Taylor expansion of the function $y_\delta(t)$ at $\delta t = 0$, allows us to express $y_\delta(t+\delta t) = y_\delta(t) + \delta t y'_\delta(t) + \frac{\delta t^2}{2} y''_\delta(t) + o(\delta t^2)$, thus Eq. (11.10) becomes,

$$\Gamma(1+\alpha)\frac{(\delta t y'_\delta(t) + \frac{\delta t^2}{2} y''_\delta(t) + o(\delta t^2))}{\delta t^\alpha} = f(y_\delta(t)). \tag{11.11}$$

Finally taking the limit $\delta t \to 0$ gives $f(y(t)) = 0$, for $0 < \alpha < 1$, and hence $y(t)$ can not be a solution of Eq. (11.1) except in the trivial case $y(t) = 0$. It follows that the discretisation given by Eq. (11.7) does not recover the original continuous equation, Eq. (11.1), in the limit of small time steps.

As an aside, we note that in the special case $\alpha = 1$, Eq. (11.11), becomes,

$$\frac{(\delta t y'_\delta(t) + \frac{\delta t^2}{2} y''_\delta(t) + o(\delta t^2))}{\delta t} = f(y_\delta(t)), \tag{11.12}$$

and hence in the limit $\delta t \to 0$ this recovers the integer order equation,

$$\frac{dy(t)}{dt} = f(y(t)). \tag{11.13}$$

Thus in this special case of $\alpha = 1$ the discretisation, Eq. (11.7), does converge to Eq. (11.1).

A numerical demonstration of the lack of convergence, for $0 < \alpha < 1$, is shown in Figure 11.1. Here we have considered the first order discretisation of the Riccati equation, Eq. (11.1) with $f(x(t)) = 1 - x(t)^2$, and show that it tends to the function $x(t) = 1$ for $t > 0$, as $\delta t \to 0$. This is consistent with the equation $f(x(t)) = 0$ as derived above.

11.4 Piecewise Constant Integrabilisation

Whilst the final result of the method described in the series of papers [49, 5, 69, 135, 47, 48, 51, 50] is incorrect, the initial approach that has been undertaken has merit. Here we will consider a correct extension of this approach for the general Caputo initial value problem given in Eq. (11.1). We will construct a family of equations, parametrized by δt such that in the limit $\delta t \to 0$ the family limits to Eq. (11.1). Each member of the family is an integrable frODE with a closed form solution. We will refer to this process as an integrablization of Eq. (11.1). Here this is achieved by replacing the right hand side of the frODE with a piecewise constant function. Choosing some time step δt, the frODE to solve would become,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t) = f\left(x\left(\delta t\left\lfloor\frac{t}{\delta t}\right\rfloor\right)\right). \tag{11.14}$$

We show below that this is an integrable equation whose solution is trivially obtained. The piecewise constant function is chosen so that in the limit of small δt we recover the original equation, i.e.

$$ \lim_{\delta t\to 0} f\left(x\left(\delta t\left\lfloor\frac{t}{\delta t}\right\rfloor\right)\right) = f(x(t)). \tag{11.15}$$

Using a unit step function, defined by

$$ u(t) = \begin{cases} 0 & t < 0, \\ 1 & t \geq 0, \end{cases} \tag{11.16}$$

we can rewrite the right-hand side Eq. (11.14) as a sum, giving

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t) = \sum_{m=0}^{\infty} f(x(m\delta t))(u(t-m\delta t) - u(t-(m+1)\delta t)). \tag{11.17}$$

The infinite sum on the right hand side of this equation is convergent as for any value t the difference between the step functions is 0 for all bar one term. Equation

(11.17) can be expressed as a sum of single unit step functions,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t) = f(x_0) + \sum_{m=1}^{\infty} \left(f(x(m\delta t)) - f(x((m-1)\delta t))\right) u(t - m\delta t). \tag{11.18} $$

The solution of this equation can be found utilising Laplace transforms. The Laplace transform of Eq. (11.18) yields,

$$ s^{\alpha}\mathcal{L}\{x(t)\} - s^{\alpha-1}x_0 = s^{-1}f(x_0) + s^{-1}\sum_{m=1}^{\infty} \left(f(x(m\delta t)) - f(x((m-1)\delta t))\right) e^{-sm\delta t}, \tag{11.19} $$

where $x(0) = x_0$. Rearranging and inverting the Laplace transform gives,

$$ x(t) = x_0 + \frac{t^{\alpha}}{\Gamma(1+\alpha)} f(x_0) + \sum_{m=1}^{\infty} \left(\frac{(t - m\delta t)^{\alpha}}{\Gamma(1+\alpha)} (f(x(m\delta t)) - f(x((m-1)\delta t))) \right) u(t - m\delta t). \tag{11.20} $$

We note that this is a solution in continuous t. This can be simplified to an n^{th} order difference equation by setting $t = n\delta t$,

$$ x(n\delta t) = x_0 + \frac{(n\delta t)^{\alpha}}{\Gamma(1+\alpha)} f(x_0) + \sum_{m=1}^{n-1} \frac{((n-m)\delta t)^{\alpha}}{\Gamma(1+\alpha)} (f(x(m\delta t)) - f(x((m-1)\delta t))). \tag{11.21} $$

This difference equation incorporates the history of the function and as such the order of the difference equation grows with each time step.

The complexity of arithmetic operations in Eq. (11.21) grows with the iteration number n. The first two terms accumulate with $\mathcal{O}(1)$, however due to the memory effect for each evaluation of a new time step n, we are required to sum over the entire history of $n-1$ terms. Hence the algorithm has $\mathcal{O}(n^2)$ arithmetic complexity.

11.5 Limit $\alpha \to 1$

Here we show that in the limit $\alpha \to 1$ that Eq. (11.21) will recover the simple Euler discretisation of an integer order ODE. Taking $\alpha = 1$, Eq. (11.21), becomes,

$$x(n\delta t) = x_0 + (n\delta t)f(x_0) + \sum_{m=1}^{n-1}((n-m)\delta t)(f(x(m\delta t)) - f(x((m-1)\delta t))). \quad (11.22)$$

Subtracting $x((n-1)\delta t)$ from both sides of this equation then yields.

$$\begin{aligned} x(n\delta t) - x((n-1)\delta t) = (n\delta t - (n-1)\delta t)f(x_0) + \sum_{m=1}^{n-1}((n-m)\delta t)(f(x(m\delta t)) \\ - f(x((m-1)\delta t))) - \sum_{m=1}^{n-2}((n-1-m)\delta t)(f(x(m\delta t)) - f(x((m-1)\delta t))). \end{aligned} \quad (11.23)$$

This simplifies to,

$$x(n\delta t) - x((n-1)\delta t) = \delta t f(x((n-1)\delta t)). \quad (11.24)$$

This is the Euler discretisation of the ODE,

$$\frac{dx(t)}{dt} = f(x). \quad (11.25)$$

11.6 Convergence

It is easy to confirm that the discretisation given in Eq. (11.21) will limit to the solution of Eq. (11.1) in the limit as $\delta t \to 0$. Firstly we note that the solution of Eq. (11.1) can be found by fractionally integrating both side of the equation giving,

$$x(t) - x(0) = \int_0^t \frac{(t-t')^{\alpha-1}}{\Gamma(\alpha)} f(x(t'))dt'. \quad (11.26)$$

Integrating by parts leads to,

$$x(t) = x(0) + \frac{t^\alpha f(x(0))}{\Gamma(1+\alpha)} + \int_0^t \frac{(t-t')^\alpha}{\Gamma(1+\alpha)} \frac{d}{dt'} f(x(t'))dt'. \tag{11.27}$$

Now considering Eq. (11.21), we can write,

$$x(n\delta t) = x_0 + \frac{(n\delta t)^\alpha}{\Gamma(1+\alpha)} f(x_0) + \sum_{m=1}^{n-1} \frac{\delta t((n-m)\delta t)^\alpha}{\Gamma(1+\alpha)} \frac{(f(x(m\delta t)) - f(x((m-1)\delta t)))}{\delta t}. \tag{11.28}$$

Taking the limit $\delta t \to 0$ such that $t = n\delta t$ and $t' = m\delta t$ are fixed then one recovers Eq. (11.27). This shows that the discretisation given in Eq. (11.21) converges to the solution of Eq. (11.1) in the limit $\delta t \to 0$. This also shows that the discretisation could have been derived from a quadrature of Eq. (11.27). This integral form representation of the method shows that this is related to a fractional order Adams method [40, 160].

11.7 Fixed Points

It is clear that any fixed points of Eq. (11.1) must also be fixed points of the discretisation given in Eq. (11.21). A point x^* is a fixed point of Eq. (11.1) provided that $f(x^*) = 0$. Consider the discretised dynamics given by Eq. (11.21) with an initial condition $x_0 = x^*$. By construction we can see that the trajectory $x(n\delta t) = x^*$ for all n and hence x^* is also a fixed point of the discretised equation. We begin by considering the point $x(\delta t)$. From Eq. (11.21) we have,

$$x(\delta t) = x^* + \frac{(n\delta t)^\alpha}{\Gamma(1+\alpha)} f(x^*), \tag{11.29}$$

$$= x^*. \tag{11.30}$$

In general for the point $x((n+1)\delta t)$ we will have,

$$x((n+1)\delta t) = x^* + \sum_{m=1}^{n} \frac{((n+1-m)\delta t)^\alpha}{\Gamma(1+\alpha)} (f(x(m\delta t)) - f(x((m-1)\delta t))), \tag{11.31}$$

and $x((n+1)\delta t) = x^*$ provided that $x(m\delta t) = x^*$ for all $m \leq n$. Thus, as $x(0) = x(\delta t) = x^*$, we have inductively shown that $x(n\delta t) = x^*$ for all $n \geq 0$. Hence any fixed point of Eq. (11.1) must also be a fixed point of Eq. (11.21).

11.7.1 Linear Stability

Next we consider the linear stability of the fixed points. Considering a small initial displacement away from the fixed point x^*, so that $x(0) = x^* + \delta x_0$. We can write the solution at some later time as $x(t) = x^* + \delta x(t)$, and using this Eq. (11.1) can be written as,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}\delta x(t) = f(x^* + \delta x(t)). \tag{11.32}$$

Performing a Taylor series expansion on the right hand side, with respect to δx about 0, and retaining the linear term gives,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}\delta x(t) = f'(x^*)\delta x(t). \tag{11.33}$$

This linear equation has a solution of the form,

$$ \delta x(t) = \delta x(0) E_{\alpha}(f'(x^*)t^{\alpha}). \tag{11.34}$$

Considering the long term behaviour of this solution if $f'(x^*) > 0$ then $x(t) \to \infty$ as $t \to \infty$ and we would say that the fixed point x^* is linearly unstable. Otherwise the point is linearly stable. Rewriting Eq. (11.14) and linearising gives,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}\delta x(t) = f'(x^*)\delta x\left(\left\lfloor \frac{t}{\delta t} \right\rfloor \delta t\right). \tag{11.35}$$

From Eq. (11.21) we see that this has a solution of,

$$ \delta x(n\delta t) = \delta x(0) + \frac{(n\delta t)^{\alpha}}{\Gamma(1+\alpha)} f'(x^*)\delta x(0) + \sum_{m=1}^{n-1} \frac{((n-m)\delta t)^{\alpha}}{\Gamma(1+\alpha)} f'(x^*)(\delta x(m\delta t) - \delta x((m-1)\delta t)). \tag{11.36}$$

We will say that the fixed points of the discrete dynamics have unchanged linear stability and are asymptotically stable if $f'(x^*) < 0$ implies that $x(n\delta t) \to 0$ as $n \to \infty$. Typically this will be expressible as a function of the step size δt. We can solve Eq. (11.36) with Z-transform techniques. Taking the Z-transform of Eq. (11.36) and rearranging we find,

$$\mathcal{Z}\left\{\delta x(n\delta t)\right\} = \frac{z^2\delta x(0)\Gamma(1+\alpha)}{(z-1)(z\Gamma(1+\alpha) - \delta t^\alpha f'(x^*)(z-1)\mathcal{Z}\left\{n^\alpha\right\})}, \tag{11.37}$$

where the Z-transform is defined as,

$$\mathcal{Z}\left\{\delta x(n\delta t)\right\} = \sum_{n=0}^{\infty} z^{-n}\delta x(n\delta t). \tag{11.38}$$

We see that in the case $f'(x^*) > 0$, $\mathcal{Z}\left\{\delta x(n\delta t)\right\}$ has a pole for $|z| > 1$, and hence $\delta x(n\delta t)$ is unbounded as $n \to \infty$. This implies that any fixed point that is unstable for the continuum dynamics will remain unstable for the discrete dynamics. For the case $f'(x^*) < 0$ we can use the Z-transform generalised final value theorem that states [56],

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=0}^{n} \delta x(i\delta t) = \lim_{z\to 1}(1-z)\mathcal{Z}\left\{\delta x(n\delta t)\right\}. \tag{11.39}$$

Note that if the sequence $\delta x(n\delta t)$ has a limit as $n \to \infty$ then $\frac{1}{n}\sum_{i=0}^{n}\delta x(i\delta t)$ will tend to the limit as $n \to \infty$. Performing the limit using Eq. (11.37) we find,

$$\lim_{z\to 1}(1-z)\mathcal{Z}\left\{\delta x(n\delta t)\right\} = 0, \tag{11.40}$$

and so,

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=0}^{n} \delta x(i\delta t) = 0. \tag{11.41}$$

This shows that if the sequence of $\delta x(n\delta t)$ tends to a limit then that limit is zero, and hence the discrete fixed point will be stable. Formally it remains to show that

$\delta x(n\delta t)$ does approach a limit as $n \to \infty$, and typically this can be achieved by considering a sufficiently small time step δt.

11.8 Non-uniform Time Step

One benefit of this approach is the ease of implementing a non-uniform time step. Non-uniform time steps can be used to concentrate time points around areas of greater change in the solution and can improve the performance of the method [90, 92]. The approximation to Eq. (11.1), can be formulated so that the time steps, $\{\delta\tau_1, \delta\tau_2 \ldots\}$, are not uniformly sized. Let the sum of the first i time steps be represented as τ_i i.e.

$$\tau_i = \sum_{j=1}^{i} \delta\tau_j. \tag{11.42}$$

With the unit step notation the frODE approximation is,

$${}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t}x(t) = f(x_0) + \sum_{m=1}^{\infty} \left(f(x(\tau_m)) - f(x(\tau_{m-1}))\right) u(t-\tau_m). \tag{11.43}$$

Again, the solution can be found using Laplace transform techniques. Following the same method as above this gives,

$$x(t) = x_0 + \frac{t^{\alpha}}{\Gamma(1+\alpha)} f(x_0) + \sum_{m=1}^{\infty} \left(\frac{(t-\tau_m)^{\alpha}}{\Gamma(1+\alpha)} (f(x(\tau_m)) - f(x(\tau_{m-1}))) \right) u(t-\tau_m). \tag{11.44}$$

This leads to a difference equation by setting $t = \tau_n$,

$$x(\tau_n) = x_0 + \frac{\tau_n^{\alpha}}{\Gamma(1+\alpha)} f(x_0) + \sum_{m=1}^{n-1} \frac{(\tau_n - \tau_m)^{\alpha}}{\Gamma(1+\alpha)} (f(x(\tau_m) - f(x((\tau_{m-1}))). \tag{11.45}$$

This difference equation reduces to Eq. (11.21) when uniform time steps are taken.

11.9 Examples

11.9.1 The Fractional Order Ricatti Equation

The fractional order Riccati equation,

$$ {}_{\mathrm{C}}D^{\alpha}_{0,t}x(t) = 1 - \rho(x(t))^2, \tag{11.46}$$

with the initial condition $x(0) = x_0$ was considered in [49], resulting in the first order difference equation approximation,

$$ x((n+1)\delta t) = x(n\delta t) + \frac{\delta t^{\alpha}}{\Gamma(1+\alpha)}(1 - \rho(x(n\delta t))^2). \tag{11.47}$$

Our discretisation of Eq. (11.46) can be found from Eq. (11.45),

$$ x(\tau_n) = x_0 - \frac{\tau_n^{\alpha}}{\Gamma(1+\alpha)}(1-\rho x_0^2) - \sum_{m=1}^{n-1} \frac{(\tau_n - \tau_m)^{\alpha}}{\Gamma(1+\alpha)}[(1-\rho(x(\tau_m))^2) - (1-\rho(x(\tau_m - 1))^2)]. \tag{11.48}$$

Taking $\tau_n = n\delta t$ leads to the fixed time step discretisation of Eq. (11.21). Figure 11.1 shows the results of these two discritization methods with $\rho = 1$, $\alpha = 0.8$, and $x_0 = 0.5$, for $\delta t = 0.1,\ 0.01$, and 0.001. From the figure, we can see that Eq. (11.47) produces a sequence that is convergent to $x(n\delta t) = 1$, i.e. $f(x(t)) = 0$ for $t > 0$, as $\delta t \to 0$. This is in contrast to the results from Eq. (11.48). We also see that the results from Eq. (11.48) display a much slower approach to the equilibrium at $x = 1$ that is characteristic of fractional order differential equations.

11.9.2 Linear Fractional Differential Equation

To show that the discretisation presented here correctly captures the dynamics of a fractional order differential equation we will consider a simple case with a known exact solution. Consider the Caputo frODE,

$$ {}_{\mathrm{C}}D^{\alpha}_{0,t}x(t) = -cx(t), \tag{11.49}$$

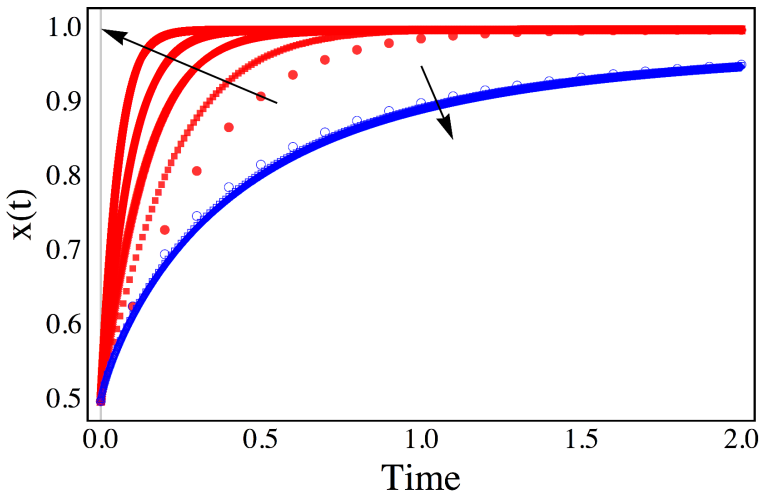

Figure 11.1: Comparison between a first order difference approximation Riccati equation [49], Eq. (11.47) for $\delta t = 0.1$, 0.01, 0.001, 0.0001, and 0.00001 (Red), and the results of the integrablization, Eq. (11.48), for $\delta t = 0.1$, 0.01, 0.001, 0.0001 (Blue). The arrows indicate the directions of decreasing δt. The first order discretisation is clearly not converging to the solution of the fractional Riccati equation.

with $x(0) = x_0$. As this is a linear equation the solution is easily found by Laplace transform methods,

$$x(t) = x_0 E_\alpha(-ct^\alpha), \tag{11.50}$$

where $E_\alpha(y)$ is a Mittag-Leffler function.

To check that the discretisation correctly captures the dynamics we will compare the exact solution with discrete points generated by the piecewise constant integrablization. We will also compare against the standard Grünwald-Letnikov discretisation of the same equation and a numerical solution found via a predictor corrector method. The Grünwald-Letnikov discretisation of Eq. (11.49) is given by,

$$x(n\delta t) = x_0 - c\delta t^\alpha x((n-1)\delta t) - \sum_{m=1}^{n-1}(-1)^m \begin{pmatrix} \alpha \\ m \end{pmatrix} (x((n-m)\delta t) - x_0)\,. \tag{11.51}$$

A more exact approximation can be formed by a predictor corrector method [41]. This involves constructing an approximation from a higher order Adams method by correcting a lower order prediction. This scheme is easy to implement, although

it does not result in a simple difference equation in the same manner as the above method. For details of the scheme see [41].

The difference equation from a piecewise constant integrablization can be found from Eq. (11.45),

$$x(\tau_n) = x_0 - \frac{c(\tau_n)^\alpha}{\Gamma(1+\alpha)}x_0 - \sum_{m=1}^{n-1}\frac{c(\tau_n-\tau_m)^\alpha}{\Gamma(1+\alpha)}(x(\tau_m)-x(\tau_{m-1})). \tag{11.52}$$

Taking $\tau_n = n\delta t$ leads to the fixed time step discretisation. As well as a fixed time step we will consider two cases of non-uniform time steps. In the first case we will draw a set of τ_n's from a uniform distribution such that the expected value of $\tau_n - \tau_{n-1}$ is δt. In the second case we deterministically chose the τ_n such that the difference between subsequent τ's is an increasing function. Again the time steps are chosen so that the average value is δt.

We define the error in the approximation $x_{\delta t}(t)$, with respect to the exact solution $x(t)$ as,

$$E(t) = |x(t) - x_{\delta t}(t)|, \tag{11.53}$$

Figure shows the results of these discretisations on the time interval $[0, 3]$, where we have taken, $\alpha = 0.5$, $c = 1$, $x_0 = 1$, and $\delta t = 0.25$. The residuals are calculated by taking the difference between the discretisation value and the exact value, i.e. $x(\tau_n) - E_\alpha(-c\tau_n^\alpha)$. For a fixed time step the Grünwald-Letnikov discretisations and piecewise constant integrablization are similar in their accuracy with the predictor corrector method providing a much better solution at the same δt. As we would expect taking a set of τ_n's that sample the dynamics more closely at earlier times, when the solution has a larger gradient, gives a better approximation for small times. The random sampling time step shows that the discretisation scheme is robust to the choice of time step.

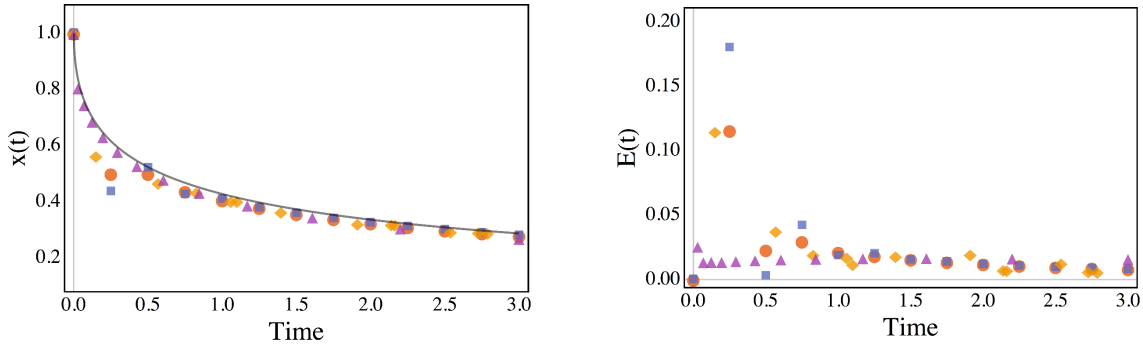

Figure 11.2: The Grünwald-Letnikov discretisation (Orange Circles) and the piecewise constant integrablization on the time interval $[0, 3]$ (Blue Squares, fixed time step, Yellow Diamonds, random time steps, and Purple Triangles, non-uniform spaced time steps) of Eq. (11.49) with $\alpha = 0.5$, $c = 1$, $x_0 = 1$, and $\delta t = 0.25$. The left panel shows the solutions, with the exact solution given as a solid black line, and the right panel shows the difference between the exact solution and the discritisation.

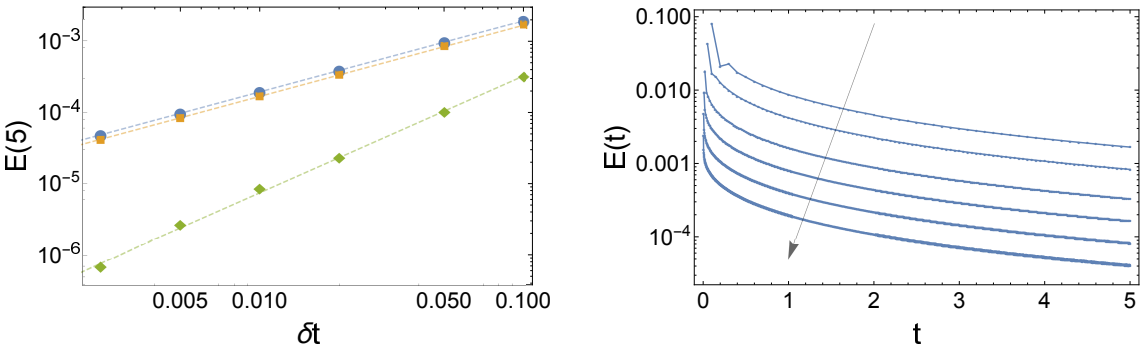

Figure 11.3: Left panel: The convergence of the numerical schemes for the linear fractional ODE. The error in the Grünwald-Letnikov discretisation (Blue Circles), the piecewise constant integrablization (Orange Squares), and the predictor-corrector method (Green Diamonds) are plotted against the time step δt. The orange and blue dashed lines have a slope of 1 whilst the green dashed line has a slope of 1.64. Right Panel: The time evolution of the error in the piecewise constant integrablization for the same δt values as the left panel. The arrow indicates the direction of decreasing δt

11.9.3 A Fractional Duffing Oscillator

We consider an undamped fractional order Duffing oscillator governed by the equation,

$$ {}_{\mathrm{C}}D^{\alpha}_{0,t}x(t) = ax(t)^3 + bx(t) + c\cos(\omega t), \tag{11.54}$$

with $1 < \alpha < 2$. As the degree of the fractional derivative is greater then one, we decompose the equation into a set of lower order differential equations. Letting $\beta = \alpha - 1$, and $y(t) = \frac{dx(t)}{dt}$, we have

$$\frac{dx(t)}{dt} = y(t), \tag{11.55}$$

$${}_{\mathrm{C}}D^{\beta}_{0,t}y(t) = ax(t)^3 + bx(t) + c\cos(\omega t). \tag{11.56}$$

This set of differential equations now involves a fractional differential equation whose order is between zero and one, and hence amenable to our integrablization. Using Eq. (11.45) to discretize the fractional equation, and the standard Euler discretisation for the integer order equation, for a fixed δt we find,

$$x(n\delta t) = x((n-1)\delta t) + \delta t y((n-1)\delta t) \tag{11.57}$$

$$\begin{aligned} y(n\delta t) =& x_0' + \frac{(n\delta t)^{\beta}}{\Gamma(1+\beta)}(ax(n\delta t)^3 + bx(n\delta t) + c\cos(\omega n\delta t)) \\ &+ \sum_{m=1}^{n-1} \frac{((n-m)\delta t)^{\beta}}{\Gamma(1+\beta)}(ax(m\delta t)^3 + bx(m\delta t) + c\cos(\omega m\delta t)) \\ &- \sum_{m=1}^{n-1} \frac{((n-m)\delta t)^{\beta}}{\Gamma(1+\beta)}(ax((m-1)\delta t)^3 + bx((m-1)\delta t) + c\cos(\omega(m-1)\delta t)), \end{aligned} \tag{11.58}$$

with $x(0) = x_0$. We can also discretize this system using a Grünwald-Letnikov derivative and the standard Euler discretisation. This gives,

$$x(n\delta t) = x((n-1)\delta t) + \delta t y((n-1)\delta t) \tag{11.59}$$

$$\begin{aligned} y(n\delta t) =& (\delta t)^{\beta}(x_0' + ax((n-1)\delta t)^3 + bx((n-1)\delta t) + c\cos(\omega(n-1)\delta t)) \\ &- \sum_{m=1}^{n-1}(-1)^m \begin{pmatrix} \beta \\ m \end{pmatrix} (y((n-m)\delta t) - x_0'), \end{aligned} \tag{11.60}$$

with $x(0) = x_0$.

Again we will also consider an approximation found via a predictor corrector method [41].

The numerical evaluation of these methods is presented in Figure 11.4, for $\alpha = 1.8$, $a = -\frac{1}{2}$, $b = 1$, $c = 2$, and $\omega = 1$. We see that both the Grünwald discretisation and the integrablization are similar in accuracy, whilst the predictor-corrector method results in a much more accurate approximation. As we do not have an exact solution to compare against, the accuracy of the predictor-corrector method can be used to give a good approximation for a ground truth solution. With a small enough time step the approximation from the predictor-corrector has a sufficiently small error so as to be negligible when compared with the errors of all the methods at larger time steps. For this ground truth solution we will take a time step of $\delta t = 2.5 \times 10^{-5}$. We define the relative error in the approximation $x_{\delta t}(t)$ then as,

$$E(t) = |x_{GT}(t) - x_{\delta t}(t)|, \tag{11.61}$$

where x_{GT} is the ground truth approximation.

The approach taken in this example of breaking a frODE whose order is greater than one into a system of equations can be applied more generally [89]. If an frODE has an order between k and $k+1$ then it can be broken down into a system of k DEs with order one, and one frODE of order between zero and one.

11.10 Summary

We have demonstrated that the first order discretisations of frODEs based on piecewise constant approximations in a series of papers [49, 5, 69, 135, 47, 48, 51, 50] do not converge to the corresponding frODE in the continuous time limit. The difference equations, being of first order, cannot capture the dynamics of the original frODE. We have presented a correct derivation of an increasing order difference equation based on a piecewise constant approximation for the vector field of the frODE. This discretisation method is amenable to non-uniform time steps and can easily be implemented on nonlinear frODEs, including non-autonomous frODEs.

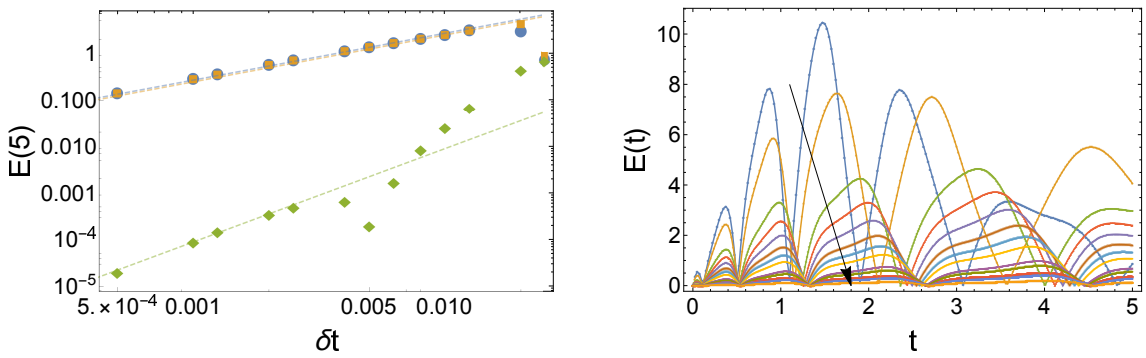

Figure 11.4: Left Panel: The error in the discretisation of the fractional Duffing oscillator, Eq. (11.54), as a function of δt. The orange squares are the integrablization, from Eqs. (11.57) and (11.58), the blue circles are the Grünwald-Letnikov discretisation, given by Eqs. (11.59) and (11.60), and the green diamonds are from a predictor corrector method. The dashed lines show that the error is scaling with δt for the integrablization and Grünwald-Letnikov discretisation, and δt^2 for the predictor corrector method. Right Panel: The error as a function of time for the integrablization for the same δt values as the left panel. The arrow indicates decreasing δt.

Whilst the method presented here is less accurate then current state of the art techniques, such as predictor-corrector type methods [41], it should be possible to adapt this scheme to obtain high order accuracy. Simply considering a piecewise polynomial interpolation rather then piecewise constant will give an improvement without overly complicating the Laplace transform techniques employed. Furthermore, it should be possible to adapt this to a predictor-corrector scheme.

Chapter 12

Piecewise Fractional PDE Method

12.1 Introduction

The work in this Chapter is based on [17] and introduces a novel method for the solution of nonlinear time-fractional partial differential equations via a semi-analytical integrabilisation method. This extends the integrabilisation method for fractional ODEs that the authors introduced in [16]. The integrabilised representation of the nonlinear fractional PDE is achieved through the construction of a one parameter family of time-integrable fractional PDEs that is consistent with the original fractional PDE in the limit of this parameter. Each member of this family of fractional PDEs is amenable to solution via Laplace transform techniques. The solution of these fractional PDEs and the subsequent discretisation of the solution forms a basis for a numerical method that may be used to approximate the solution of the original fractional PDE.

This approach to the construction of a numerical method for a fractional PDE differs from traditional approaches in that we construct an approximation for the entire equation rather then any single operator. In fact at no stage do we discretise the fractional derivative in constructing our method. We show that our method is somewhat similar to an Adams method, in that it can be seen to be equivalent to a quadrature of a fractional integral.

In the following we will consider fractional PDEs involving Caputo derivatives, however the method can readily be extended to other fractional derivatives. We de-

velop the Piecewise Constant Integrabilisation in Section 12.2 and we have provided a general convergence result. As a simple application we consider the fractional heat equation in Section 12.3. Exact solutions for the fractional heat equation are found considering polynomial initial conditions on an unbounded domain. In this application we show that the integrabilisation is exact for cubic in space initial conditions, but is only an approximation for higher polynomial order initial conditions. In Section 12.4 we turn our attention the fractional diffusion-wave equation using the time integrabilisation with a spectral solution of the spatial derivatives. We also provide a stability result for the spectral integrabilisation in this application. In Section 12.5 we show how the integrabilisation behaves for the integer order time derivative in the non-linear Burgers' equation. We conclude with summary remarks in Section 12.6.

12.2 Piecewise Constant Integrabilisation

Here we consider an initial value fractional PDE,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t} w(x,t) = \rho\left(x,t,w(x,t)\right), \tag{12.1} $$

for $\alpha > 0$, where $\rho(x,t,w(x,t))$ is a function of x,t and a spatial operator on $w(x,t)$. In order to create piecewise constant integrabilisation of this fractional PDE, we extend the previously considered piecewise constant method for fractional ODEs [15]. To begin we replace the right hand side of the fractional PDE, Eq. (12.1), with a piecewise constant function in t. We choose a δt such that,

$$ {}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t} w(x,t) = \rho\left(x, \left(\delta t \left\lfloor \frac{t}{\delta t} \right\rfloor\right), w\left(x, \delta t \left\lfloor \frac{t}{\delta t} \right\rfloor\right)\right). \tag{12.2} $$

As we take the limit of $\delta t \to 0$ we recover the original equation, since,

$$ \lim_{\delta t \to 0} \rho\left(x, \left(\delta t \left\lfloor \frac{t}{\delta t} \right\rfloor\right), w\left(x, \delta t \left\lfloor \frac{t}{\delta t} \right\rfloor\right)\right) = \rho\left(x,t,w(x,t)\right). \tag{12.3} $$

The right hand side of this equation can be rewritten using a unit step function, defined by,

$$u(t) = \begin{cases} 0 & t < 0, \\ 1 & t \geq 0. \end{cases} \tag{12.4}$$

Then the right hand side becomes,

$${}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t} w(x,t) = \sum_{m=0}^{\infty} \rho\left(x, (m\delta t), w(x, m\delta t)\right) \left(u(t - m\delta t) - u(t - (m+1)\delta t)\right). \tag{12.5}$$

By considering a change of limits this can be rewritten as a sum of unit step functions,

$$\begin{aligned} &{}_{\mathrm{C}}\mathcal{D}^{\alpha}_{0,t} w(x,t) = \rho\left(x, 0, w(x,0)\right) \\ &+ \sum_{m=1}^{\infty} \left(\rho\left(x, (m\delta t), w(x, m\delta t)\right) - \rho\left(x, (m-1)\delta t, w(x, (m-1)\delta t)\right)\right) u(t - m\delta t). \end{aligned} \tag{12.6}$$

Equation (12.6) can be solved by using a Laplace transform with respect to time. Using the Laplace transform definition from Eq. (1.11) we arrive at,

$$\begin{aligned} &s^{\alpha}\mathcal{L}\{w(x,t)\} - \sum_{k=0}^{n-1} s^{\alpha-k-1} w^{(0,k)}(x,0) = s^{-1}\rho\left(x, 0, w(x,0)\right) \\ &+ s^{-1} \sum_{m=1}^{\infty} \left(\rho\left(x, (m\delta t), w(x, m\delta t)\right) - \rho\left(x, (m-1)\delta t, w(x, (m-1)\delta t)\right)\right) e^{-sm\delta t}. \end{aligned} \tag{12.7}$$

Here, we have defined $w^{(i,j)}(x_0, t_0)$ to be the mixed ith derivative with respect to x and the jth derivative with repect to t of $w(x,t)$ evaluated at (x_0, t_0), i.e.,

$$w^{(i,j)}(x_0, t_0) = \left.\frac{\partial^{i+j} w(x,t)}{\partial x^i \partial t^j}\right|_{x=x_0, t=t_0}. \tag{12.8}$$

Rearranging and inverting the Laplace transform gives,

$$w(x,t) = \sum_{k=0}^{n-1} w^{(0,k)}(x,0)\frac{t^k}{k!} + \rho\left(x,0,w(x,0)\right)\frac{t^\alpha}{\Gamma(\alpha+1)}$$
$$+ \sum_{m=1}^{\infty}\left(\rho\left(x,(m\delta t),w(x,m\delta t)\right) - \rho\left(x,(m-1)\delta t,w(x,(m-1)\delta t)\right)\right)\frac{(t-m\delta t)^\alpha}{\Gamma(\alpha+1)}u(t-m\delta t). \tag{12.9}$$

This is the exact solution of Eq. (12.2). As such the solution is defined for all time t.

To obtain a numerical method we must discretise time. Considering the time points $t = l\delta t$ the solution becomes,

$$w(x,l\delta t) = \sum_{k=0}^{n-1} w^{(0,k)}(x,0)\frac{(l\delta t)^k}{k!} + \rho\left(x,0,w(x,0)\right)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)}$$
$$+ \sum_{m=1}^{l-1}\left(\rho\left(x,(m\delta t),w(x,m\delta t)\right) - \rho\left(x,(m-1)\delta t,w(x,(m-1)\delta t)\right)\right)\frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \tag{12.10}$$

Notice that no information was lost in going from Eq. (12.9) to Eq. (12.10). Knowing the solution at the discrete time points, $t = l\delta t$, is sufficient to construct the solution at any other time.

Equation (12.10) forms the basis of our numerical method, although, depending on the form of the function $\rho(x,t,w(x,t))$, further spatial discretisation may be required. In most cases standard finite difference operators may be used to deal with integer order spatial derivatives. It may also be possible to avoid a spatial discretisation by finding a spectral solution of the equation. We will look at specific examples of these different approaches in the examples, but first we obtain a general convergence result.

12.2.1 Convergence

We check that our discretisation in Eq. (12.10) limits to the solution of Eq. (12.1) in the limit as $\delta t \to 0$, by considering the integral of both equations. To begin we

integrate Eq. (12.1) with respect to t, yielding,

$$w(x,t) - \sum_{k=0}^{n-1} w^{(0,k)}(x,0)\frac{t^k}{k!} = \int_0^t \frac{(t-t')^{\alpha-1}}{\Gamma(\alpha)}\rho\left(x,t',w(x,t')\right)dt'. \tag{12.11}$$

Integrating by parts leads to,

$$\begin{aligned} w(x,t) =& \sum_{k=0}^{n-1} w^{(0,k)}(x,0)\frac{t^k}{k!} \\ &+ \frac{t^\alpha \rho\left(x,0,w(x,0)\right)}{\Gamma(\alpha+1)} + \int_0^t \frac{(t-t')^\alpha}{\Gamma(\alpha+1)}\frac{d}{dt'}\rho\left(x,t',w(x,t')\right)dt'. \end{aligned} \tag{12.12}$$

Turning to Eq. (12.10), we can express it as,

$$\begin{aligned} w(x,l\delta t) =& \sum_{k=0}^{n-1} w^{(0,k)}(x,0)\frac{(l\delta t)^k}{k!} + \rho\left(x,0,w(x,0)\right)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} \\ &+ \sum_{m=1}^{l-1} \frac{\delta t((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)} \frac{\left(\rho\left(x,(m\delta t),w(x,m\delta t)\right) - \rho\left(x,(m-1)\delta t,w(x,(m-1)\delta t)\right)\right)}{\delta t}. \end{aligned} \tag{12.13}$$

Taking the limit $\delta t \to 0$ such that $t = l\delta t$ and $t' = m\delta t$ then one recovers Eq. (12.12). This shows that the discretisation given in Eq. (12.10) converges to the solution of Eq. (12.1) in the limit $\delta t \to 0$. This also shows that the discretisation could have been derived from a quadrature of Eq. (12.12).

12.3 Fractional Heat Equation

We consider the classic heat equation,

$$\frac{\partial}{\partial t}w(x,t) = \frac{\partial^2}{\partial x^2}w(x,t), \tag{12.14}$$

with the first order derivative replaced by a fractional time derivative,

$${}_C\mathcal{D}^\alpha_{0,t}w(x,t) = \frac{\partial^2}{\partial x^2}w(x,t), \tag{12.15}$$

here we have restricted ourselves to $0 < \alpha \leq 1$. The integrablization present above approximates Eq. (12.15) as,

$$w(x, l\delta t) = w(x, 0) + w^{(2,0)}(x, 0)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} + \sum_{m=1}^{l-1} \left(w^{(2,0)}(x, m\delta t) - w^{(2,0)}(x, (m-1)\delta t)\right) \frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \quad (12.16)$$

By considering an initial condition that is polynomial in space on an unbounded domain we can construct both exact solutions to the fractional heat equation, Eq. (12.15), and the integrablization, Eq. (12.16).

12.3.1 Integrablization of the Fractional Heat Equation

If we assume an initial condition that is a polynomial in x of degree p without boundaries, then we may express solutions of Eq. (12.16) without any spatial discretisation. As the RHS of the equation involves only the function, and second derivatives of the function, from earlier times, then the polynomial initial condition ensures that the solution at all later times may be written as a polynomial of degree p with respect to x so that,

$$w(x, l\delta t) = \sum_{i=0}^{p} a_i(l\delta t)x^i. \quad (12.17)$$

Substituting this into Eq. (12.16) then gives,

$$\sum_{i=0}^{p} a_i(l\delta t)x^i = \sum_{i=0}^{p} a_i(0)x^i + \sum_{i=0}^{p-2}(i+1)(i+2)a_{i+2}(0)x^i\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} + \sum_{m=1}^{l-1}\left(\sum_{i=0}^{p-2}(i+1)(i+2)\left(a_{i+2}(m\delta t) - a_{i+2}((m-1)\delta t)\right)x^i\right)\frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \quad (12.18)$$

Matching coefficients leads to equations for the time evolution of each of the polynomial coefficients. The highest two degree coefficients are unchanging in time,

$$a_p(l\delta t) = a_p(0) \tag{12.19}$$

$$a_{p-1}(l\delta t) = a_{p-1}(0) \tag{12.20}$$

All other coefficients are evolved by the relation,

$$\begin{aligned} a_i(l\delta t) = a_i(0) + (i+1)(i+2)a_{i+2}(0)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} \\ + \sum_{m=1}^{l-1}\left((i+1)(i+2)\left(a_{i+2}(m\delta t) - a_{i+2}((m-1)\delta t)\right)\right)\frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \end{aligned} \tag{12.21}$$

As an example, we consider an initial condition that is quadratic in x, i.e. $w(x,0) = a_0(0) + a_1(0)x + a_2(0)x^2$. For such an initial condition Eq. (12.16) has the solution,

$$w(x, l\delta t) = a_0(0) + 2a_2(0)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} + a_1(0)x + a_2(0)x^2. \tag{12.22}$$

12.3.2 Exact Solution of the Fractional Heat Equation

The procedure used in Section 12.3.1 can be followed in general to obtain exact solutions to Eq. (12.15) for any initial condition that is a polynomial in x. Again, in general, given a polynomial initial condition of degree p then the solution at all times can be written as a polynomial of degree p, i.e.

$$w(x,t) = \sum_{i=0}^{p} a_i(t)x^i. \tag{12.23}$$

The integral form of the solution to the fractional heat equation can be found from Eq. (12.12),

$$w(x,t) = w(x,0) + \frac{t^\alpha w^{(2,0)}(x,0)}{\Gamma(\alpha+1)} + \int_0^t \frac{(t-t')^\alpha}{\Gamma(\alpha+1)} w^{(2,1)}(x,t')dt'. \tag{12.24}$$

Substituting the polynomial representation of the solution into this equation and then matching coefficients we find that the two highest order coefficients are constant in time, i.e.

$$a_p(t) = a_p(0) \tag{12.25}$$

$$a_{p-1}(t) = a_{p-1}(0). \tag{12.26}$$

We also see that the remaining coefficients are given by the following equation,

$$a_i(t) = a_i(0) + \frac{(i+1)(i+2)a_{i+2}(0)t^\alpha}{\Gamma(\alpha+1)} + \int_0^t \frac{(t-t')^\alpha}{\Gamma(\alpha+1)}(i+1)(i+2)a_{i+2}^{(1)}(t')dt'. \tag{12.27}$$

As the coefficients $a_p(t)$ and $a_{p-1}(t)$ are constant in time it is possible to express the coefficients as polynomials in t^α. Explicitly,

$$a_i(t) = \sum_{j=0}^{\lfloor \frac{p-i}{2} \rfloor} \frac{\Gamma(1+i+2j)a_{i+2j}(0)t^{j\alpha}}{\Gamma(1+i)\Gamma(1+j\alpha)}. \tag{12.28}$$

From this we can write down the exact solution of the fractional heat equation via the sum in Eq. (12.23),

$$w(x,t) = \sum_{i=0}^{p} \left(\sum_{j=0}^{\lfloor \frac{p-i}{2} \rfloor} \frac{\Gamma(1+i+2j)a_{i+2j}(0)t^{j\alpha}}{\Gamma(1+i)\Gamma(1+j\alpha)} \right) x^i. \tag{12.29}$$

This solution can be checked explicitly by substituting into the fractional heat equation, Eq. (12.15).

12.3.3 Comparison Between the Exact Solution and the Integrablization of the Fractional Heat Equation

Returning to the case of a quadratic initial condition it is trivial to see that the solution of the integrablization, Eq. (12.22), matches the exact solution, Eq. (12.29), for all $t = l\delta t$. For initial conditions that are polynomials in x of degree greater then three the integrablization solution will not exactly match the solution given in Eq.

(12.29). The evolution of the highest four polynomial coefficients, i.e. $a_p(t)$, $a_{p-1}(t)$, $a_{p-2}(t)$, and $a_{p-3}(t)$, will always be exact regardless of the order p.

To examine this difference we will consider a numerical example. We take an initial condition of the polynomial formed from a finite truncation of the Taylor series expansion of $\exp(x - x^2)$ about 0, for example for $p = 5$ this would be

$$w(x, 0) = 1 + x - \frac{x^2}{2} - \frac{5x^3}{6} + \frac{x^4}{24} + \frac{41x^5}{120}. \tag{12.30}$$

The exact and integrablization polynomial coefficients were solved under a range of δt values with $\alpha = 0.8$. The solutions were compared over the interval $x \in [-1, 1]$ by integrating the absolute value of the difference between the two solutions to produce an absolute L_1 error, $E(\delta t, t)$. The relative error, $R(\delta t, t)$, is defined as the absolute error divided by the integral of the exact solution over $x \in [-1, 1]$. The results are presented in Figure 12.1. From this figure we see that the error grows unbounded in time, this is to be expected as the exact solution also grows unbounded in time. For the case $p = 5$ we also see a convergence of $O(\delta t)$.

12.4 Fractional Diffusion-Wave Equation

This example considers the linear diffusion-wave equation, which in the integer order case is given by,

$$\frac{\partial^2}{\partial t^2} w(x, t) = \frac{\partial^2}{\partial x^2} w(x, t). \tag{12.31}$$

This equation is almost identical to the heat equation, differing only by the order of the time derivative. We will use a formulation for which Agrawal has provided exact solutions on a bounded domain [6]. The time fractional version of this equation is given by

$${}_C\mathcal{D}^{\alpha}_{0,t} w(x, t) = \frac{\partial^2}{\partial x^2} w(x, t), \tag{12.32}$$

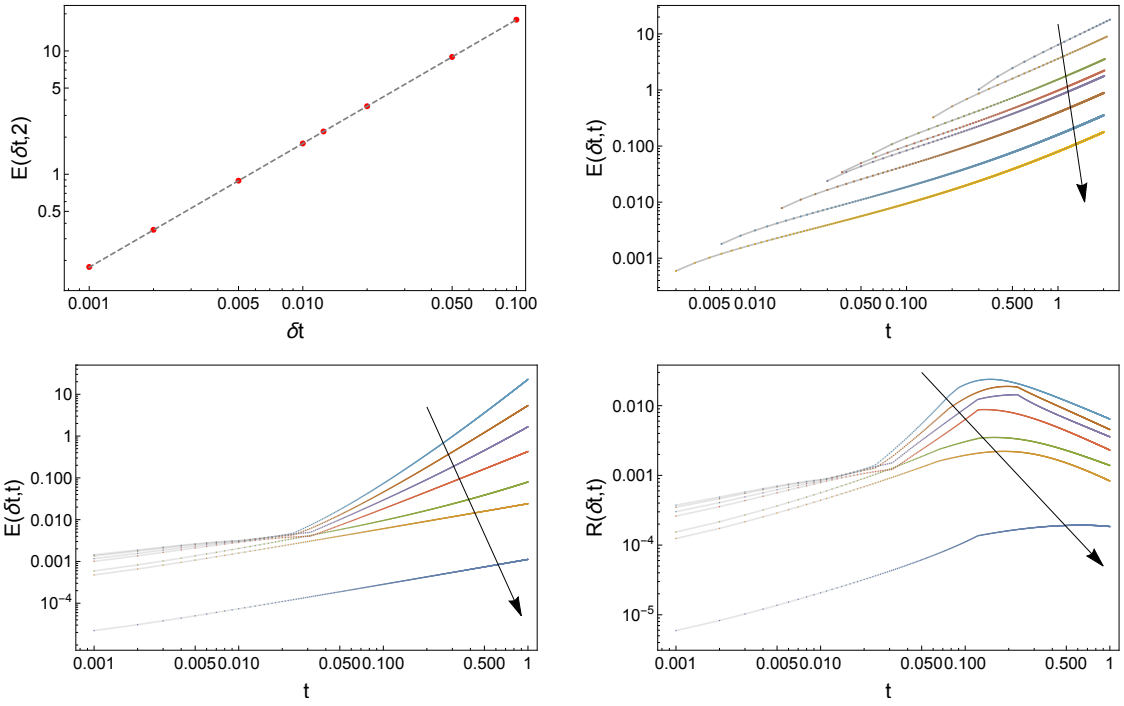

Figure 12.1: The error in the integrablization of the fractional heat equation given initial conditions given in by a Taylor series of $\exp(x - x^2)$ about $x = 0$ of order p. Top left: The absolute error as a function of δt for $p = 6$ evaluated at $t = 2$. The dashed line is a linear best fit in δt. Top right: The evolution of the absolute error as a function of time. The arrow indicates decreasing δt. Bottom left: The time evolution of the absolute error for $p = 4, 5, 6, 7, 8, 9, 10$, at fixed $\delta t = \frac{1}{1000}$. The arrow indicates decreasing p. Bottom right: The time evolution of the relative error for $p = 4, 5, 6, 7, 8, 9, 10$, at fixed $\delta t = \frac{1}{1000}$. The arrow indicates decreasing p.

with $1 < \alpha \leq 2$, subject to the initial conditions

$$w(x,0) = \begin{cases} x & 0 \leq x \leq 1, \\ 2 - x & 1 \leq x \leq 2, \end{cases} \tag{12.33}$$

and

$$w^{(0,1)}(x,0) = 0. \tag{12.34}$$

We now impose Dirichlet boundary conditions

$$w(0,t) = w(2,t) = 0. \tag{12.35}$$

Applying the present method yields

$$w(x,l\delta t) = w(x,0) + w^{(0,1)}(x,0)(l\delta t) + w^{(2,0)}(x,0)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} + \sum_{m=1}^{l-1}\left(w^{(2,0)}(x,m\delta t) - w^{(2,0)}(x,(m-1)\delta t)\right)\frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \tag{12.36}$$

12.4.1 Spectral Solution of the Integrablization

As an alternative to the standard finite difference approach we can form a spectral method by considering the evolution of single Fourier components. As we have imposed zero value Dirichlet boundary conditions on Eq. (12.32) we will assume that its solution can be expressed as a sine decomposition on the interval $x \in [0,2]$, this gives,

$$w\left(x,t\right) = \sum_{n=0}^{\infty}\sigma_n(t)\sin\left(\frac{\pi}{2}nx\right). \tag{12.37}$$

This representation makes the calculation of the second derivative in x trivial,

$$w^{(2,0)}\left(x,t\right) = \sum_{n=0}^{\infty}-\sigma_n(t)\left(\frac{\pi}{2}n\right)^2\sin\left(\frac{\pi}{2}nx\right). \tag{12.38}$$

Due to the linear nature of Eq. (12.32) we only need to consider the evolution of a single wave number n. Simplifying Eq. (12.36) with the above assumptions then gives,

$$\sigma_n(l\delta t) = \sigma_n(0) + \sigma_n^{(1)}(0)(l\delta t) - \left(\frac{\pi}{2}n\right)^2\sigma_n(0)\frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} + \sum_{m=1}^{l-1}\left(\sigma_n((m-1)\delta t) - \sigma_n(m\delta t)\right)\left(\frac{\pi}{2}n\right)^2\frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \tag{12.39}$$

Any initial condition, $f(x)$, that obeys zero valued Dirichlet boundary conditions may also be represented by a Fourier sine decomposition,

$$f(x) = \sum_{n=0}^{\infty}\sigma_n(0)\sin\left(\frac{\pi}{2}nx\right), \tag{12.40}$$

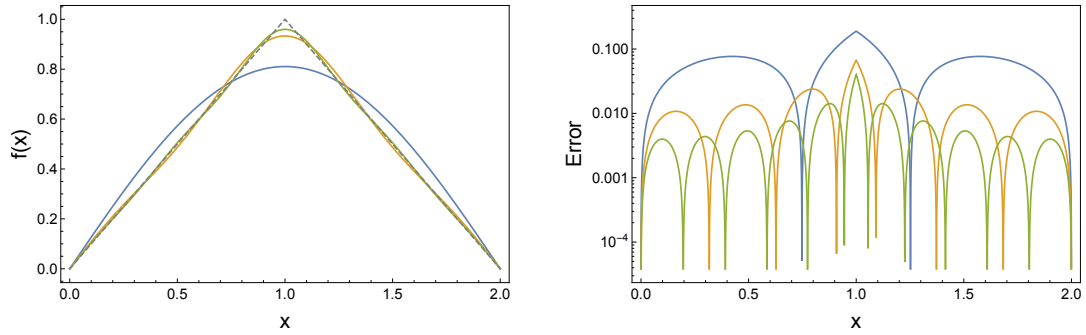

Figure 12.2: The spectral representation of the initial condition for the fractional wave equation. Left: The spectral representation of the initial condition function, $f(x)$, for maximum wavenumbers up to $n = 1$, 5, and 10. The dashed line is the exact function. Right: The difference between the exact initial condition function and its spectral representation with maximum wavenumbers up to $n = 1$, 5, and 10.

where

$$\sigma_n(0) = \int_0^2 f(x) \sin(\frac{\pi}{2} nx)\, dx. \tag{12.41}$$

Any initial conditions imposed on higher order derivatives may be similarly. In our case, Eq. (12.34) gives the trivial condition $\sigma_n^{(1)}(0) = 0$.

Thus the fractional wave equation, posed in Eq. (12.32), can be approximated by evolving a finite set of wave numbers according to Eq. (12.39), subject to the initial condition given by Eq. (12.41).

The accuracy of the solution will be limited to the accuracy of the representation of the initial condition. Taking a finite number of wave numbers to represent the initial condition given in Eq. (12.33) will always result in a loss of information. The accuracy of the finite Fourier decomposition is captured in Fig. (12.2), illustrating the qualitative shape of the initial condition and the absolute difference.

12.4.1.1 Stability

For a given δt we observe that the evolution of the solution for a finite number of wavenumbers is stable. In order to capture higher spatial frequencies a smaller time step is required. Due to the sum over the past history the standard Fourier stability analysis is complicated and results in inequalities that are not readily reducible to easy to interpret conditions. Instead we will consider a different limit found

by considering the evolution of the solution. We know that the analytic solution requires that $|\sigma_n(t)| < |\sigma_n(\tau)|$ for all $t > \tau$. Moreover we also know that evolution should not change the sign of $\sigma_n(t)$, i.e. if $\sigma_n(\tau) > 0$ then $\sigma_n(t) > 0$ for all $t > \tau$. Thus if $\sigma_n(0) > 0$ the method will be unstable if $\sigma_n(l\delta t) < 0$ for any $l > 0$. This gives us an instability criteria from Eq. (12.39),

$$\begin{aligned} 0 > \sigma_n(0) - \left(\frac{\pi n}{2}\right)^2 \sigma_n(0) \frac{(l\delta t)^\alpha}{\Gamma(\alpha+1)} + \\ \sum_{m=1}^{l-1} \left(\sigma_n((m-1)\delta t) - \sigma_n(m\delta t)\right) \left(\frac{\pi n}{2}\right)^2 \frac{((l-m)\delta t)^\alpha}{\Gamma(\alpha+1)}. \end{aligned} \tag{12.42}$$

If we assume that $\sigma_n(k\delta t) > 0$ for all $0 \leq k < l$ then $(\sigma_n((m-1)\delta t) - \sigma_n(m\delta t)) > 0$ for all $m > 1$. This reduces our instability criteria to the more manageable,

$$\frac{n^2\pi^2(l\delta t)^\alpha}{4\Gamma(\alpha+1)} > 1. \tag{12.43}$$

If this is not true for any l if it is not true for $l = 1$. This implies that, given a δt, our method is unstable for the evolution of the solution of wavenumbers where,

$$n > \left(\frac{4\Gamma(\alpha+1)}{\pi^2(\delta t)^\alpha}\right)^{\frac{1}{2}}. \tag{12.44}$$

12.4.2 Comparison Between the Exact Solution and the Spectral Integrablization

We numerically solve the intergablisation to compare with the exact solution. Following Agrawal [6], the exact solution to Eq. (12.32) given the initial conditions by Eqs. (12.33) and (12.34), subject to the boundary conditions Eq. (12.35), is given by the infinite series,

$$w_e(x,t) = \sum_{n=1}^{\infty} E_\alpha(-\frac{\pi^2 n^2}{4} t^\alpha) \sin(\frac{n\pi}{2} x) \left(\frac{8\sin(\frac{n\pi}{2}) - 4\sin(n\pi)}{n^2\pi^2}\right). \tag{12.45}$$

For the purposes of computation we truncate the series when the terms become less then 10^{-9}. The spectral integrablization is computed by considering a finite

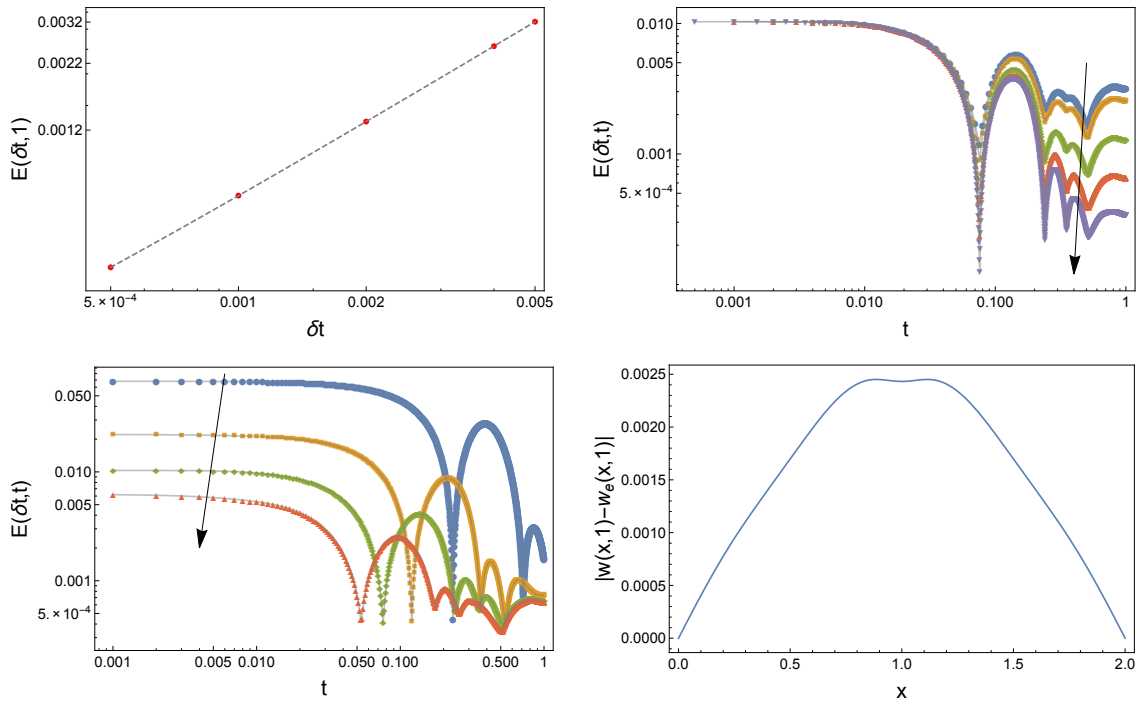

Figure 12.3: The error in the spectral solution of the integrablization of the fractional wave equation given a piecewise linear initial condition. Top left: The absolute error as a function of δt for a spectral solution at time $t = 1$ taking wavenumbers up to $n = 5$. The dashed line is a linear best fit in δt. Top right: The evolution of the absolute error as a function of time of a spectral solution taking wavenumbers up to $n = 5$. The arrow indicates decreasing δt. Bottom left: The time evolution of the absolute error for the spectral solution taking wavenumbers up to $n = 1, 3, 5, 7$, at fixed $\delta t = \frac{1}{1000}$. The arrow indicates decreasing maximum wavenumber n. Bottom right: The difference between the exact solution and the spectral integrablisation across the domain with $n = 5$ at $t = 1$.

truncation of the sum in Eq. (12.37). Each of the required $\sigma_n(l\delta t)$ functions were computed via Eq. (12.39). We considered the case of $\alpha = \frac{3}{2}$ and the results are presented in Fig. (12.3). Here we can see a linear convergence rate of the solution as $\delta t \to 0$.

12.5 Burgers' Equations

We now consider the integer order nonlinear Burgers' equation due to the availability of an exact solution to which we may compare our numerical scheme. The equation is given by,

$$\frac{\partial w(x,t)}{\partial t} + w(x,t)\frac{\partial}{\partial x}w(x,t) = \nu\frac{\partial^2}{\partial x^2}w(x,t). \tag{12.46}$$

In the infinite domain case the Burgers' equation is satisfied by the following equation,

$$w(x,t) = 1 + 2\nu \tanh(c + t - x). \tag{12.47}$$

As we wish to consider a finite domain we implement time dependent Dirichlet boundary conditions on the domain $x \in [0, L]$. Taking the boundary conditions of the form,

$$w(0,t) = 1 + 2\nu \tanh(c + t), \tag{12.48}$$

$$w(L,t) = 1 + 2\nu \tanh(c + t - L), \tag{12.49}$$

ensures that the infinite domain exact solution, Eq. (12.47), is also a solution for our finite domain problem. Here we set $L = 10$, $c = 0$ and $\nu = 1/2$. Using standard finite difference approximations to the spatial derivatives, the integrablization, Eq. (12.10), applied to Brugers' equation gives,

$$\begin{aligned} w(i\delta x, l\delta t) &= w(i\delta x, 0) + \rho\left(i\delta x, 0, w(i\delta x, 0)\right)(l\delta t) \\ &+ \sum_{m=1}^{l-1} \left(\rho\left(i\delta x, (m\delta t), w(x, m\delta t)\right) - \rho\left(i\delta x, (m-1)\delta t, w(i\delta x, (m-1)\delta t)\right)\right)((l-m)\delta t), \end{aligned} \tag{12.50}$$

for $0 < i < L/\delta x$, where

$$\begin{aligned} \rho(i\delta x, l\delta t, w(i\delta x, l\delta t)) = \Bigg(\nu \left(\frac{w((i+1)\delta x, l\delta t) - 2w(i\delta x, l\delta t) + w((i-1)\delta x, l\delta t)}{\delta x^2}\right) \\ - w(i\delta x, l\delta t)\frac{w((i+1)\delta x, l\delta t) - w((i-1)\delta x, l\delta t)}{2\delta x}\Bigg). \end{aligned} \tag{12.51}$$

From Eq. (12.50) we can easily see that,

$$w(i\delta x, l\delta t) - w(i\delta x, (l-1)\delta t) = \delta t \rho\left(i\delta x, (l-1)\delta t, w(i\delta x, (l-1)\delta t)\right). \tag{12.52}$$

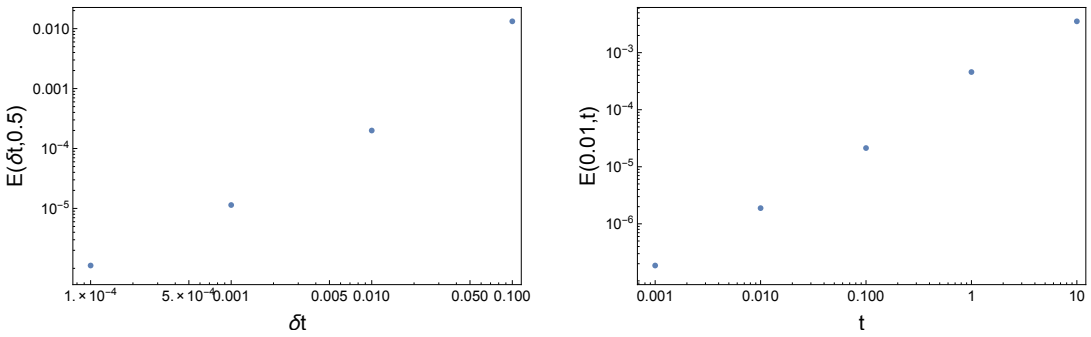

Figure 12.4: The error in the solution of the integrablization of Burgers' equation. Left: The absolute error as a function of δt for the solution at time $t = 0.5$.Right: The evolution of the L_1 error as a function of time with $\delta t = 0.01$ and $\delta x = 0.1$.

This shows that when $\alpha = 1$ the sum over the history of the function is not required and we recover a simple Euler method as a time discretization. For completeness and in comparison to the non-integer order case we will numerically evaluate this scheme. The values of δx are chosen so that $M = L/\delta x$ is an integer. The boundary conditions are implemented numerically by fixing the value of the numerical function at the boundaries of the domain. This gives,

$$w(0, l\delta t) = 1 + 2\nu \tanh(c + l\delta t), \tag{12.53}$$

$$w(M\delta x, l\delta t) = 1 + 2\nu \tanh(c + l\delta t - M\delta x). \tag{12.54}$$

The initial condition is also taken from Eq. (12.47),

$$w(i\delta x, 0) = 1 + 2\nu \tanh(c - i\delta x). \tag{12.55}$$

Figure 12.4 illustrates, numerically, the increase in accuracy of the numerical scheme as δt and δx are decreased. This numerically validates the convergence discussion given in Section 12.2.1. Figure 12.4 also shows the time evolution of the L_1 error, $E(\delta t, t)$. The initial increase with time is due to the wave-front passing through the domain.

12.6 Summary

We have introduced a new method for enabling the time integration of nonlinear time-fractional partial differential equations. The method does not provide a discretisation of the fractional derivative but instead it uses a integrablization of the fractional PDE.

The method presented in this Chapter is an extension to the work on fractional ODEs in [15] to fractional PDEs. The introduction of a spatial domain presents a host of approaches to the solution of the spatially dependent fractional PDE as has been discussed above. The stability of the proposed scheme is dependent on the relationship between δt and δx and we note that with a rigorous stability criterion one could adaptively choose δt, as is done in [15], to reduce the computational time of the method.

Several numerical examples are given as a means of illustrating the efficacy and accuracy of the proposed method for linear and nonlinear PDEs and fractional PDEs on both bounded and unbounded domains. In addition to this a convergence proof is provided which validates the proposed method.

Chapter 13

Thesis Summary and Discussion

Over the past few decades there has been increased interest in developing fractional-order models, both ODE and PDE. This is due to the history effect that fractional-order derivatives introduce into the system. However without sufficient care *ad hoc* fractional-order models can have non-physical parameters or a violation of flux-balance. By deriving fractional-order models from an underlying stochastic process, physical fractional-order models can be derived. This thesis presents the derivation of both fractional-order ODEs and PDEs which can be used as mathematical models. This body of work has firmly established the use of CTRWs in the development of fractional-order models.

In Part I we focused on the derivation of fractional-order ODE models. This began by deriving stochastically consistent fractional SIR models and a more general fractional-order compartment model and concluded with discrete formulations of our continuous models, providing a stable numerical scheme to solve the equations. In doing so, we presented the conditions under which fractional-order derivatives arise. This is a novel approach to fractional-order ODEs.

Part II was centred around the derivation of fractional-order PDEs. Whilst these derivations are significant in their own right, they also raise considerations around underlying stochastic processes. These considerations include; the non-unique stochastic framework which can result in the same equations; and the different ways in which 'forces' can be introduced.

Part III described a novel numerical approach for solving fractional ODEs and PDEs based on piecewise approximations and integrabilisations.

The use of the CTRW as a stochastic process from which once could derive physically consistent fractional-order ODEs and fractional-order PDEs was reliant on the introduction of power-law tailed waiting time densities such as the Mittag-Leffler density. The use of exponential waiting time densities results in integer order derivatives.

The key difference between the exponential and Mittag-Leffler distributions is that the former is memoryless. For the exponential distribution the 'waiting time' until the next jump is not dependent on how much time has already elapsed. In the case of the Mittag-Leffler distribution the longer that one has waited, the longer one expects to wait. This memory property, the memory of how much time one has already waited, becomes manifest through a fractional derivative in the governing evolution equation. The fractional derivative, like an integral, requires the knowledge of the full history of the solution, but unlike an integral it expresses the time rate of change of this full history, and it applies different weighting to different parts of the history.

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