

# Mixed Discrete–Continuous Fragmentation Equations



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Dedicated to my mother Anne Baird. Without her love, belief, encouragement and support I would not be where I am today and I deeply wish she were here to witness this submission.

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# Abstract

The work contained in this thesis concerns the development, and the mathematical and numerical analysis, of a new class of hybrid discrete–continuous fragmentation model. The framework is introduced as a potential answer to the occurrence of ‘shattering’ mass loss, commonly observed in purely continuous fragmentation models.

Initially, the study begins by introducing the model, which takes the form of an integro-differential equation, coupled with a system of ordinary differential equations. Once the model has been established, it is subjected to a rigorous mathematical analysis, using the theory and methods of operator semigroups and their generators. Most notably, by applying the theory relating to the Kato–Voigt perturbation theorem, honest substochastic semigroups and operator matrices, the existence of a unique, differentiable solution to the model is established. This solution is also shown to preserve non-negativity and conserve mass.

Having determined the existence of a solution, the work continues with the development of a numerical scheme for the approximate solution of the modelling equations. Considering a truncated version of the equations, rewritten in an alternative conservative form, the scheme is built around a finite volume discretisation. Using a standard weak compactness argument, the approximations generated by the numerical scheme are shown to converge (weakly) to a weak solution of the truncated equations.

By relating this weak solution to the strong solutions provided by the earlier semigroup analysis, the weak solution is found to be unique and as a consequence, differentiable, non-negative and mass-conserving. The theoretical study is completed with an examination of the effect of varying the truncation point. In particular, establishing that as the length of the truncated interval is increased, in the limit, the original solution to the full model is obtained.

Finally, the thesis is completed with a numerical investigation, seeking to experimentally confirm the assertions of the earlier theoretical work and assess the performance of the numerical scheme for a suite of test models.

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# Chapter 1

## Introduction

Coagulation and fragmentation processes are common phenomena, occurring in many physical systems. They arise in many diverse areas, such as colloidal chemistry [79], polymer science [83], population dynamics [23], biology [12] and astrophysics [39]. The mathematical models of such processes typically classify the particles within the system according to some physical state variable, for example their volume, area or mass, the aim is then to determine the evolution of the system with respect to this variable as time progresses. Models are typically classified as either discrete or continuous, depending on the nature of the state variable of interest.

### 1.1 Coagulation and Fragmentation Models

The first mathematical model of such a process was provided by Smoluchowski in [79]. It concerns the case of binary coagulation amongst particles with discrete size, that is where all particles are composed of integer multiples of some base monomer. The model consists of the following infinite set of nonlinear differential equations:

$$\frac{du(t)_i}{dt} = \frac{1}{2} \sum_{j=1}^{i-1} k_{i-j,j} u(t)_{i-j} u(t)_j - u(t)_i \sum_{j=1}^{\infty} k_{i,j} u(t)_j, \quad i = 1, 2, \dots \quad (1.1)$$

The functions  $u(t)_i$  give the concentration of  $i$ -sized ( $i \in \mathbb{N}$ ) particles at time  $t$ . The values  $k_{i,j}$  are the coagulation kernels and give the rates at which  $i$  and  $j$ -sized particles join to form one of size  $i + j$ . The nature of the process demands that these values are non-negative and symmetric, i.e.  $k_{i,j} = k_{j,i}$ . The first term on the right of (1.1) is a gain term and accounts for the increase in  $i$ -sized particles when two suitably sized smaller particles coalesce. The  $\frac{1}{2}$  appearing in front of this term is included so as to avoid double counting. The second term is a loss term corresponding to the loss of  $i$ -sized particles when such a particle joins with any other.

A continuous analogue of (1.1) was introduced by Müller in [62]. Here particle size becomes a continuous variable as opposed to the discrete values appearing in (1.1). This model takes the form of an integro-differential equation:

$$\frac{\partial u(x, t)}{\partial t} = \frac{1}{2} \int_0^x k(x-y, y) u(x-y, t) u(y, t) dy - u(x, t) \int_0^\infty k(x, y) u(y, t) dy. \quad (1.2)$$

The unknown function  $u(x, t)$  represents the particle density for size  $x$  at time  $t$ , so that  $u(x, t) dx$  gives the average number of particles whose size lies within the interval  $(x, x + dx)$  at time  $t$ . Similarly to before, the coagulation kernel  $k(x, y)$  provides the rate at which a particle of size  $x$  and another of size  $y$  join. The interpretation of terms in (1.2) correspond with those of (1.1). Despite Smoluchowski providing only the discrete model, both (1.1) and (1.2) are known as the Smoluchowski coagulation equation.

The literature abounds with work on the Smoluchowski coagulation equations, with many results on the existence of solutions and their properties for various classes of coagulation  $k(x, y)$ . For an overview of this material the reader is advised to examine the reviews by Drake [25], Aldous [2], Laurençot and Mischler [52] and more recently Niethammer [67] and the references therein. The table below sets out some concrete examples of coagulation kernels which appear in the literature, as well as the setting in which they are applied. This table is based on one appearing in [2], which itself is taken from [77], where the associated references may be found. A similar outline for the discrete equation (1.1) can be found in [22].

Coagulation Kernels	
$k(x, y)$	Application
$(x^{1/3} + y^{1/3})(x^{-1/3} + y)$	Brownian motion (continuum regime)
$(x^{1/3} + y^{1/3})^2(x^{-1} + y^{-1})^{1/2}$	Brownian motion (free molecular regime)
$(x^{1/3} + y^{1/3})^3$	Shear (linear velocity profile)
$(x^{1/3} + y^{1/3})^{7/3}$	Shear (nonlinear velocity profile)
$(x^{1/3} + y^{1/3})^2 \left  x^{1/3} - y^{1/3} \right $	Gravitational settling
$(x^{1/3} + y^{1/3})^2 \left  x^{2/3} - y^{2/3} \right $	Inertia and gravitational settling
$(x-y)^2(x+y)^{-1}$	Analytic approximation of Berry's kernel
$(x+c)(y+c)$	Branched-chain polymerisation
$(x^{1/3} + y^{1/3})(xy)^{1/2}(x+y)^{-3/2}$	Based on kinetic theory

Table 1.1: Example kernels and their applications.

The models above describe a pure coagulation process. We can introduce a reverse, fragmentation, process whereby particles may break-up into smaller pieces. In the

continuous case, the first to consider such a model was Melzak [60], who introduced a special case of the following coagulation–fragmentation equation:

$$\frac{\partial u(x, t)}{\partial t} = -u(x, t) \int_0^x \frac{y}{x} \gamma(x, y) dy + \int_x^\infty \gamma(y, x) u(y, t) dy + (\mathcal{C}u)(x, t), \quad (1.3)$$

where  $\mathcal{C}u$  represents the coagulation terms from the right-hand side of equation (1.2). The fragmentation kernel  $\gamma(x, y)$ ,  $0 \leq y \leq x < \infty$ , provides the rate at which particles of size  $y$  are produced from the break-up of a particle of size  $x$ . Therefore, the first term on the right-hand side of equation (1.3) is interpreted as a loss term, which takes account of the particles of size  $x$  which are lost when such particles break into smaller pieces. Conversely, the second term is a gain term, accounting for the increase in particles of size  $x$  arising from the fragmentation of larger particles.

A special case of the fragmentation model (1.3), is that of binary fragmentation. As the name suggests, in binary fragmentation, each fragmentation event results in exactly two child particles. The fragmentation equation (1.3), is readily modified to model such a process by setting

$$\gamma(x, y) = F(x - y, y), \quad 0 \leq y \leq x < \infty.$$

The function  $F(x, y)$  is the binary fragmentation kernel, and provides the rate at which particles of size  $x + y$  fragment to produce two particles of size  $x$  and  $y$ . As such, it is necessary that  $F$  is symmetric. If we replace the kernel  $\gamma(x, y)$  in the first term of (1.3) with  $F(x - y, y)$ , and make the substitution  $y' = x - y$ , we obtain

$$\int_0^x \frac{y}{x} \gamma(x, y) dy = \int_0^x \frac{y}{x} F(x - y, y) dy = \int_0^x \frac{x - y'}{x} F(y', x - y') dy'.$$

Utilising the symmetry of  $F$ , we may re-arrange this to give

$$\int_0^x \frac{2y}{x} F(x - y, y) dy = \int_0^x \frac{x}{x} F(x - y, y) dy,$$

which leads us to

$$\int_0^x \frac{y}{x} \gamma(x, y) dy = \int_0^x \frac{y}{x} F(x - y, y) dy = \frac{1}{2} \int_0^x F(x - y, y) dy.$$

Making this change in (1.3), along with an obvious replacement of the second term, gives us the following binary coagulation and binary fragmentation equation:

$$\frac{\partial u(x, t)}{\partial t} = -\frac{1}{2}u(x, t) \int_0^x F(x - y, y) dy + \int_0^\infty F(x, y)u(x + y, t) dy + (\mathcal{C}u)(x, t). \quad (1.4)$$

We note that by setting  $k \equiv 0$  in either (1.3) or (1.4), we lose the coagulation term  $\mathcal{C}u$  resulting in a pure fragmentation equation.

Within the more recent literature, the continuous multiple fragmentation equation has commonly taken an alternative form to that given in (1.3), being written instead as:

$$\frac{\partial u(x, t)}{\partial t} = -a(x)u(x, t) + \int_x^\infty a(y)b(x|y)u(y, t) dy. \quad (1.5)$$

Here the function  $a(x)$  provides the fragmentation rate for a particle of size  $x$ , whilst  $b(x|y)$  represents the distribution of the resulting particle size  $x$  conditional on the break-up of a particle of size  $y$ . Clearly as no individual particle resulting from a fragmentation event can have a size exceeding that of the original particle, we require that  $b(x|y) = 0$  for  $x > y$ . As with (1.3), the first term on the right-hand side of (1.5) is the loss term, whilst the integral term is the gain term. In order that matter be conserved during fragmentation events we must impose the following condition on the function  $b(x|y)$ :

$$\int_0^y xb(x|y) dx = y \text{ for } y > 0. \quad (1.6)$$

This condition mathematically states that the total size of all resulting particles taken together must be equal to the size of the original fragmenting particle. As (1.3) and (1.5) are in fact equivalent, we may recover our original multiple fragmentation equation by setting

$$a(x) = \int_0^x \frac{y}{x} \gamma(x, y) dy \quad \text{and} \quad b(x|y) = \frac{\gamma(y, x)}{a(y)},$$

and likewise the binary fragmentation equation by setting

$$a(x) = \frac{1}{2} \int_0^x F(x - y, y) dy \quad \text{and} \quad b(x|y) = \frac{F(y - x, x)}{a(y)}.$$

An equation of the type (1.5) was first considered by McGrady and Ziff in [57], where they sought explicit solutions in the particular case of  $a$  and  $b$  taking the following power-law forms:

$$a(x) = x^\alpha, \quad \alpha \in \mathbb{R}, \quad \text{and} \quad b(x|y) = (\nu + 2) \frac{x^\nu}{y^{\nu+1}}, \quad -2 < \nu \leq 0. \quad (1.7)$$

Fragmentation processes may also be modelled using discrete models. The discrete analogue of the fragmentation equation (1.5) is given by

$$\frac{du(t)_i}{dt} = -a_i u(t)_i + \sum_{j=i+1}^{\infty} a_j b_{i,j} u(t)_j, \quad i = 1, 2, \dots \quad (1.8)$$

As with equation (1.1),  $u(t)_i$  represents the concentration of  $i$ -sized particles at time  $t$ . The values  $a_i$  are the rates at which  $i$ -sized particles fragment, so necessarily  $a_1 = 0$ . The values  $b_{i,j}$  give the expected number of  $i$ -sized particles which are produced when one of size  $j$  breaks up. Conservation concerns impose a discrete equivalent of condition (1.6) on the choice of  $b_{i,j}$ . If we were to include the terms from the right-hand side of (1.1) we would obtain a discrete coagulation–fragmentation equation. As was the case with the continuous fragmentation models, there is a choice of ways in which to mathematically represent a discrete fragmentation process, with discrete analogues of equations (1.3) and (1.4). The first study of a discrete model of fragmentation is generally credited to Simha [75], where he examined a case of binary fragmentation which can be obtained by setting

$$a_i = \begin{cases} 0 & \text{for } i = 1 \\ 1 & \text{otherwise} \end{cases} \quad \text{and } b_{i,j} = \frac{2}{j-1}.$$

In this particular model all particle sizes are equally likely to fragment and each fragmentation event produces two resulting particles, with all admissible size pairings being equally probable.

A noteworthy case of a discrete coagulation–fragmentation equation is provided by the Becker–Döring equations. These represent a model of discrete binary coagulation and binary fragmentation where all particle resizing events must involve a monomer. That is, each coagulation event consists of a monomer joining with some other particle, whilst after any fragmentation event at least one of the two resulting particles must be a monomer. These equations take their name from the authors of the paper [13], however they considered a simplified model in which the concentration of monomers was assumed to be constant. The Becker–Döring equations as we know them now, without this simplification, appeared independently in [17] and [71], with a significant contribution coming in [7] and the follow up [6], with the first general existence and uniqueness results. Recent works on these equations [70], [64], [66] and [65] have considered the large-time behaviour of solutions and their link to other significant equations in the field of materials science.

## 1.2 Application of Semigroups

A variety of approaches have been used in the analysis of coagulation–fragmentation equations, but one route which has proved particularly successful, and which we will be extensively utilising, is the theory and results concerning operator semigroups. The first application of semigroup theory to the field of coagulation–fragmentation equations was by Aizenman and Bak [1]. They considered the case

of the binary coagulation–fragmentation equation, (1.4), under the assumption that the rates  $F$  and  $k$  are constant. The approach they adopted involved taking a sequence of approximating problems, whereby the mass variable  $x$  was restricted to a sequence of truncated intervals. Each of these truncated problems was shown to give rise to a semigroup and the resulting sequence of semigroups was shown to converge to a limit semigroup. Finally this limit semigroup was shown to provide a solution to the full problem.

Using a similar truncation/limit approach, McLaughlin *et al.* [59] were able to establish the existence of a unique, non-negative, mass-conserving solution to the pure multiple fragmentation equation, under the constraint

$$\int_0^x \frac{y}{x} \gamma(x, y) dy \leq C_n < \infty \quad \text{for all } x \in (0, n], \quad n > 0,$$

where the sequence of constants  $\{C_n\}$ , is permitted to be unbounded. This work was extended in [58] to the coagulation and multiple fragmentation equation, under the assumptions that the coagulation kernel  $k$  is constant and the multiple fragmentation kernel  $\gamma$  is bounded.

In [46], Lamb considers the coagulation and multiple fragmentation equation where the fragmentation terms are of the form of (1.5). Using the truncation/limit technique, existence and uniqueness of solutions is established under the constraints that the fragmentation rate  $a$  satisfies a linear growth bound, the coagulation kernel  $k$  is bounded and the quantity  $n(y) = \int_0^y b(x|y) dy$ , which gives the expected number of particles resulting from the fragmentation of a particle of size  $y$ , is equal to a finite constant.

A recent development in this area has been the application of the Kato–Voigt perturbation theorem [81]. It was first applied by Banasiak in [8], to a particular case of the fragmentation equation (1.5), and more generally by Lamb [46] and Banasiak and Arlotti [10] to establish the existence of unique mass-conserving positive solutions to equation (1.5) under suitable constraints on the fragmentation rate  $a$ . This approach has proved particularly fruitful and has been applied to a range of coagulation–fragmentation models, for example in [11, 12, 15, 56, 78].

### 1.3 Weak Compactness Arguments

Another approach which has been widely applied in the analysis of coagulation–fragmentation equations involves the applications of weak compactness arguments to establish the existence of solutions. The first use of such an approach is widely credited to Stewart [80], who considered the binary coagulation–fragmentation equation (1.3), proving existence of solutions under the restriction that the kernels

$k$  and  $F$  satisfy certain ‘almost linear’ growth bounds. As with the truncation/limit semigroup method mentioned in the previous section, this approach involves the approximation of our equation by a sequence of equations on finite truncated intervals, each of which is shown to have a solution. The family of solutions this gives rise to is shown to be weakly compact in a suitable  $L_1$  space. From this weak compactness, we may deduce the convergence of a subsequence of this family to some limit, with this limit then being shown to provide a solution (in some sense) to the original equation. Since [80], the approach has been utilised by a number of authors, each considering various coagulation–fragmentation problems, under a range of conditions on the kernels, for example; [49, 50, 34, 18, 33, 48].

The weak compactness style argument has also been applied to the convergence analysis of numerical schemes for coagulation–fragmentation problems. However, instead of considering a family of truncated equations, we are concerned with a sequence of discretised approximating equations and their solutions. Applying the same weak compactness argument to this family of approximations yields the convergence of the numerical scheme. Such an approach was used in [16, 44, 42].

## 1.4 Shattering

As we have seen, a range of models exist to represent coagulation and fragmentation processes. In particular when selecting a model we face a choice of whether a discrete or continuous model would be most appropriate. This selection depends largely on the scale of the phenomenon to be described and the level of detail we wish to include in our model. When the size of any fundamental base unit of matter is small compared to the overall size of a typical particle, then a continuous model may provide a satisfactory representation of reality. However if our model is to include particles on the scale of the fundamental base unit then a discrete model may be more appropriate. Further, we can encounter difficulties with continuous models when the fragmentation rate blows up at zero and particles are allowed to get too small too quickly. The unbounded fragmentation rate can result in a runaway fragmentation process and a loss of mass unaccounted for in the model formulation. This loss of mass was observed by McGrady and Ziff in [57], the process was termed ‘shattering’ and attributed to the creation of ‘dust’ particles with zero size but positive mass.

In [38], Huang *et al.* suggest that such a runaway fragmentation process is unphysical, and that at some point particles become too small to break-up any further. Their proposed model includes a cut-off size  $x_c$ , above which particles are able to fragment as usual. However, once a particle’s size drops below  $x_c$  it ceases to be able to fragment, becoming dormant. This leads to a dual state model. Particles of size  $x > x_c$ , which lie above the cut-off, form a ‘fragmentation state’. If we denote the density of particles within this regime by  $u_F(x, t)$ , then the evolution

is governed by the standard multiple fragmentation equation:

$$\frac{\partial u_F(x, t)}{\partial t} = -a(x)u_F(x, t) + \int_x^\infty a(y)b(x|y)u_F(y, t) dy, \quad x > x_c, \quad t > 0. \quad (1.9)$$

Particles of mass below the cut-off, that is those whose mass lies in the range  $0 < x \leq x_c$  form a ‘dust regime’; we denote by  $u_D(x, t)$  the density of particles in this regime. The dust regime density is then governed by the adapted fragmentation equation:

$$\frac{\partial u_D(x, t)}{\partial t} = \int_{x_c}^\infty a(y)b(x|y)u_F(y, t) dy, \quad 0 < x \leq x_c, \quad t > 0, \quad (1.10)$$

where no loss occurs. In [38], the above system was examined in the particular case where  $a$  and  $b$  are as given in (1.7). The authors provided explicit solutions to the system of equations, these solutions being given in terms of the confluent hypergeometric function. We note that the above model can be obtained from the standard equation (1.5) by setting the fragmentation rate to be zero over the interval  $(0, x_c]$ .

We propose an alternative solution to the problem in the form of a hybrid discrete/continuous model. The smallest particles in the system are modelled using a discrete model whilst those larger particles, with size above some cut-off, are modelled by a continuous model.

An analogous mass loss may occur with coagulation models in a process known as ‘gelation’. This corresponds to the creation of an infinitely sized ‘gel’ particle which is unaccounted for in our calculations and results in a breakdown in the conservation of mass within finite time. The time  $t$  at which this mass loss first occurs is known as the gelation time. This phenomenon was first observed for specific cases of coagulation equations [29, 53, 54, 85], and there now exists a large body of work attempting to answer in which cases mass-conserving solutions can be found, or when gelation occurs.

## 1.5 Numerical Analysis of C–F Equations

The models introduced above have exact solutions for a limited number of special cases, and in most examples we must resort to an appropriate numerical method in order to obtain a solution. A range of numerical techniques have been applied to these problems, and these broadly fall into two categories: those involving a stochastic (Monte Carlo) element and those based around deterministic approximation schemes. The introductory chapter of [44] and the references therein provide an overview of a number of these approximation methods.

In particular we are interested in the application of finite volume schemes for the solution of coagulation and fragmentation equations. Such methods have found common application in the solution of conservation laws and many of the models introduced above can be rewritten in such a form, usually with mass as the conserved quantity. Filbet and Laurençot [31] were the first to apply these methods in the area of coagulation and fragmentation equations, where they used such a scheme to solve a conservative formulation of (1.2). However, this article mainly involved the numerical investigation of a number of specific cases and did not include any in-depth analysis of the convergence of the scheme. This was extended by Bourgade and Filbet to include binary fragmentation in the article [16], where they applied the method to an alternative formulation of (1.4). In this paper, the scheme developed is shown to converge under suitable restrictions on the coagulation and fragmentation kernels. The particular model we shall be examining is a variation of the multiple fragmentation equation (1.5). In [44, 42], finite volume schemes are applied to reformulations of the multiple fragmentation equation (1.5) and also the corresponding coagulation–fragmentation equation. These served as a guide during the development of the numerical scheme for our own model, which includes fragmentation terms of the form (1.5). Recently, the finite volume method has been applied to coagulation–fragmentation models involving additional nucleation and particle growth processes [73, 43, 45].

## 1.6 Outline

The purpose of this thesis is to detail the original work conducted during our study. The body of the work is formed by four main chapters, however prior to this, in Chapter 2, we cover all the mathematical preliminaries required in the subsequent chapters which may be deemed non-standard. The original material is then set out as follows.

In Chapter 3 we introduce our new mixed discrete–continuous fragmentation model. Using results from the theory of semigroups, we prove, under certain restrictions on the fragmentation rate  $a$ , the existence of a unique, positive, mass-conserving solution to our model.

As mentioned previously, the majority of fragmentation models require numerical techniques to obtain a solution. In Chapter 4, we introduce a numerical scheme for the solution of a truncated version of the mixed model from Chapter 3. We then go on to establish a number of properties of solutions provided by this scheme.

In Chapter 5, we establish the weak convergence of the numerical solutions developed in Chapter 4 to a weak solution of the truncated problem introduced earlier in that same chapter.

In Chapter 6, we prove that under the assumptions in place, any weak solution to our truncated problem must correspond to the strong/classical solution of the truncated problem that would be obtained utilising the methods of Chapter 3. Finally, we consider the truncated solutions and show that in the limit, as we lengthen the truncated interval, we obtain the full solutions as we had in Chapter 3.

We complete the thesis with a numerical study in Chapter 7, where we examine a range of mixed fragmentation models using our numerical scheme and confirm the behaviour expected from our previous analysis.

# Chapter 2

## Preliminaries: Spaces, Operators and Semigroups

In this chapter we provide an introduction to the terminology and theory utilised in the later chapters. A complete cataloguing of all the mathematics used in the thesis would prove rather lengthy, and therefore we have tried to restrict attention to the material which may be deemed non-standard. In making this classification we are assuming the reader is acquainted with the basic concepts and results of functional analysis, as covered in an introductory course, such as that provided by [41, Chapters 1 and 2]. We also assume an elementary knowledge of measure theory and integration such as covered in [55, Chapter 1].

### 2.1 Spaces, Norms and Convergence

Much of the analysis conducted in the later chapters is carried out within the setting of a number of function spaces. These are chosen as a result of their applicability to our problem. In this section we introduce the family of spaces that we shall be working in extensively, and detail their key properties as far our interests are concerned.

**Definition 2.1.1.** (Lebesgue spaces) Let  $(\Omega, \mathcal{A}, \mu)$  be a measure space with positive measure  $\mu$ . For  $1 \leq p < \infty$ , we denote by  $L_p(\Omega, \mu)$  the set of (equivalence classes of)  $\mu$ -measurable (real-valued) functions  $f$  defined almost everywhere on  $\Omega$ , such that

$$\|f\|_p := \left\{ \int_{\Omega} |f(x)|^p d\mu(x) \right\}^{\frac{1}{p}} < \infty. \quad (2.1)$$

When the choice of the measure is clear, typically in the case where we are using the standard Lebesgue measure, then it is common to write  $L_p(\Omega)$  in place of  $L_p(\Omega, \mu)$ . With the expression (2.1) as a norm, the space  $L_p(\Omega, \mu)$  ( $1 \leq p < \infty$ )

forms a Banach space, [74, Theorem 3.11]. For our applications, we shall be primarily interested in cases with  $p = 1$ .

As a limiting case of this family, by  $L_\infty(\Omega, \mu)$  we denote the set of (equivalence classes of)  $\mu$ -measurable (real-valued) functions  $f$  defined almost everywhere on  $\Omega$ , for which there exists a finite constant  $M$  such that

$$|f(x)| \leq M \text{ for almost all } x \in \Omega. \quad (2.2)$$

A norm may be defined on  $L_\infty(\Omega, \mu)$  as follows:

$$\|f\|_\infty := \inf \{M : |f(x)| \leq M \text{ for } \mu\text{-almost all } x \in \Omega\}.$$

With  $\|f\|_\infty$  as a norm, the space  $L_\infty(\Omega, \mu)$  constitutes a Banach space [74, Theorem 3.11].

**Lemma 2.1.2.** *Let  $\Omega$  be open and  $1 \leq p < \infty$ ; then the space of infinitely differentiable functions with compact support  $C_c^\infty(\Omega)$  is dense in  $L_p(\Omega)$ .*

*Proof.* See [20, Theorem 7.25]. □

**Definition 2.1.3.** Suppose that  $f \in L_1(\mathbb{R}^n, \lambda)$ , where  $\lambda$  denotes the Lebesgue measure on  $\mathbb{R}^n$ . Then any point  $x \in \mathbb{R}^n$ , such that

$$\lim_{r \searrow 0} \frac{1}{\lambda(B(x, r))} \int_{B(x, r)} |f(y) - f(x)| \, d\lambda(y) = 0,$$

is called a *Lebesgue point* of  $f$ , where  $B(x, r)$  denotes the open ball of radius  $r$  centred at  $x$ .

**Theorem 2.1.4.** (Lebesgue differentiation theorem) *For  $f \in L_1(\mathbb{R}^n, \lambda)$ , almost every  $x \in \mathbb{R}^n$  is a Lebesgue point of  $f$ .*

*Proof.* See [74, Theorem 7.7]. □

**Definition 2.1.5.** For  $1 \leq p < \infty$  ( $p = \infty$ ) the space  $L_{p,loc}(\Omega)$  consists of the set of functions  $f$  which satisfy the condition (2.1) ((2.2)) on all compact subsets  $K \subset \Omega$ . Such functions are known as *p-locally integrable* functions.

**Definition 2.1.6.** Let  $X$  be a vector space of real-valued functions defined with domain  $\Omega$ . The subset  $X_+$ , is defined as

$$X_+ = \{f \in X : f(x) \geq 0 \text{ for all } x \in \Omega\},$$

and is known as the *positive cone* of  $X$ .

- (i) If the space  $X$  is of the type  $L_p$ , then the condition  $f(x) \geq 0$  for all  $x \in \Omega$  is replaced by  $f(x) \geq 0$  for  $\mu$  almost all  $x \in \Omega$ ;

- (ii) The positive cone is closed under addition and multiplication by non-negative (real) scalars;
- (iii) The positive cone of an  $L_p$  space forms a closed subset of  $L_p$ .

*Proof.* The second of these properties is self-apparent. In the case of  $L_1$  which is of most interest to us, the third property can be seen as a consequence of the upcoming Lemma 2.1.16 and Lemma 2.1.12 (iv).  $\square$

The introduction of the positive cone imposes an additional ordering structure to the space which leads to the idea of a *Banach lattice*. We do not delve into this beyond the following definition, however the interested reader may examine [10, Section 2.2] for further explanation.

**Definition 2.1.7.** A Banach lattice  $X$  forms a *KB-Space* (*Kantorovič–Banach space*) if every non-decreasing norm bounded sequence of elements from  $X_+$  converges in the norm on  $X$ .

- (i) Spaces of type  $L_1(\Omega, \mu)$  form *KB-Spaces*.

*Proof.* See [3, Theorem 12.26] and [10, Theorem 2.83].  $\square$

**Definition 2.1.8.** Let  $X_1$  and  $X_2$  be two vector spaces. The *product space*  $X = X_1 \times X_2$ , is defined as the set of ordered pairings

$$X_1 \times X_2 = \{(f, g) : f \in X_1, g \in X_2\}.$$

- (i) If  $(X_1, \|\cdot\|_{X_1})$  and  $(X_2, \|\cdot\|_{X_2})$  are both Banach spaces, then so is the product space  $X = X_1 \times X_2$ , equipped with norm

$$\|(f, g)\|_X = \|f\|_{X_1} + \|g\|_{X_2} \quad \text{for } f \in X_1, g \in X_2;$$

see [14, Lemma 1.62].

- (ii) When  $X_1$  and  $X_2$  are vector spaces of real-valued functions, then we define the positive cone of the product space  $X$  to be  $X_+ = X_{1+} \times X_{2+}$ .

**Definition 2.1.9.** Let  $X$  be a vector space and let both  $\|\cdot\|$  and  $\|\cdot\|_0$  satisfy the conditions to be norms on  $X$ . The norms are said to be *equivalent* if there exist positive constants  $a$  and  $b$  such that

$$a\|f\| \leq \|f\|_0 \leq b\|f\| \quad \text{for all } f \in X.$$

Equivalent norms define the same topology on  $X$ ; hence notions of convergence which are defined with respect to such norms are equivalent. We say that the normed spaces  $(X, \|\cdot\|)$  and  $(X, \|\cdot\|_0)$  are equivalent.

**Theorem 2.1.10.** *In the analysis pursued in subsequent chapters we shall be working extensively in spaces of the type  $L_1$ . In particular we shall be working in the spaces  $L_1 = L_1((N, R) \times [0, T], dx dt)$  and  $L_1^1 = L_1((N, R) \times [0, T], x dx dt)$ , where  $N$  is a positive integer and  $R > N$  is a finite real value. With the associated norms, these form equivalent spaces as described in Definition 2.1.9.*

*Proof.* First let us suppose that  $f \in L_1^1$ ; then we have

$$\|f\|_{L_1} = \int_0^T \int_N |f(x, t)| dx dt \leq \frac{1}{N} \int_0^T \int_N |f(x, t)| x dx dt = \frac{1}{N} \|f\|_{L_1^1}.$$

Therefore  $f \in L_1$  also, with  $\|f\|_{L_1} \leq \frac{1}{N} \|f\|_{L_1^1}$ . Now let us assume that  $f \in L_1$ ; then we have

$$\|f\|_{L_1^1} = \int_0^T \int_N |f(x, t)| x dx dt \leq R \int_0^T \int_N |f(x, t)| dx dt = R \|f\|_{L_1}.$$

Hence  $f \in L_1^1$  with  $\|f\|_{L_1^1} \leq R \|f\|_{L_1}$ . Taken together, the above results show us that the spaces  $L_1((N, R) \times [0, T], dx dt)$  and  $L_1((N, R) \times [0, t], x dx dt)$  contain the same elements and have equivalent norms.  $\square$

This result shall prove useful in the analysis contained in later chapters, allowing us to switch spaces when mathematically convenient whilst retaining convergence.

Given a sequence  $\{f_n\}_{n=1}^\infty$  in a normed vector space  $(X, \|\cdot\|)$ , we assume the reader is familiar with the concept of convergence with respect to the norm  $\|\cdot\|$ , which is known as *strong* convergence. In many situations this condition is too restrictive for our purposes and we may consider other notions of convergence.

**Definition 2.1.11.** Let  $(X, \|\cdot\|)$  be a normed vector space with dual space  $X'$ . A sequence  $\{f_n\}_{n=1}^\infty \subset X$  converges *weakly* to  $f \in X$  if

$$l(f_n) \rightarrow l(f) \quad \text{as } n \rightarrow \infty, \quad \text{for all } l \in X'.$$

We denote this by  $f_n \rightharpoonup f$  and call  $f$  the *weak* limit of  $\{f_n\}$ .

**Lemma 2.1.12.** *A weakly convergent sequence  $\{f_n\}_{n=1}^\infty \subset X$  and its limit  $f$  have the following properties:*

- (i) The weak limit  $f$  of  $\{f_n\}_{n=1}^\infty$  is unique;
- (ii) Every subsequence of  $\{f_n\}_{n=1}^\infty$  converges weakly to  $f$ ;
- (iii) The sequence  $\{\|f_n\|\}_{n=1}^\infty$  is bounded;
- (iv) Strong convergence implies weak convergence with the same limit. The converse is not generally true except in the case that  $\dim(X) < \infty$ ; then weak convergence implies strong convergence.

*Proof.* See [41, Lemma 4.8-3 and Theorem 4.8-4].  $\square$

**Lemma 2.1.13.** (*Lower semicontinuity of norms*) For  $1 \leq p < \infty$  the  $L_p$ -norm is weakly lower semicontinuous, that is, given a sequence  $\{f_n\}_{n=1}^\infty$  which converges weakly to  $f$  in  $L_p(\Omega)$ , then

$$\|f\|_p \leq \liminf_{n \rightarrow \infty} \|f_n\|_p.$$

*Proof.* See [55, Theorem 2.11].  $\square$

The normed spaces we shall be utilising are of the type  $L_p(\Omega, \mu)$ . The following theorem characterises weak convergence in such a setting.

**Theorem 2.1.14.** Let  $1 \leq p < \infty$  with  $q$  such that  $1/p + 1/q = 1$  ( $q = \infty$  when  $p = 1$ ) and consider  $L_p(\Omega, \mu)$  with  $\mu$  a  $\sigma$ -finite measure, then  $\{f_n\}_{n=1}^\infty \subset L_p(\Omega, \mu)$  converges weakly to  $f \in L_p(\Omega, \mu)$  if and only if

$$\int_{\Omega} f_n g \, d\mu \rightarrow \int_{\Omega} f g \, d\mu, \quad \text{as } n \rightarrow \infty,$$

for every  $g \in L_q(\Omega, \mu)$ .

*Proof.* See [32, Section 2.1.4].  $\square$

In our analysis when handling weakly convergent sequences we will usually find them appearing alongside other factors and we would like the product to converge weakly also. The following theorem gives us sufficient conditions for the product of two sequences to converge weakly and will be used extensively in the convergence proofs for our numerical schemes.

**Theorem 2.1.15.** Let  $(\Omega, \mathcal{A}, \mu)$  be a measure space with  $\mu$  finite. Suppose  $f_n \rightharpoonup f$  in  $L_1(\Omega, \mu)$ ,  $g_n \rightarrow g$  point-wise  $\mu$  a.e. in  $\Omega$ , and  $\sup_n \|g_n\|_{L^\infty} < \infty$ , then  $f_n g_n \rightharpoonup f g$  in  $L_1(\Omega, \mu)$ .

*Proof.* [32, Proposition 2.61]  $\square$

The numerical scheme developed in the later chapters will be seen to produce a sequence of non-negative functions  $\{f_n\} \subset L_1(\Omega, \mu)_+$  which converges weakly to  $f$  in  $L_1(\Omega, \mu)$ . We would like this limit to preserve the non-negativity of the sequence. That is we would hope that the positive cone of  $L_1(\Omega, \mu)$  is a closed subset under taking weak limits. The following lemma gives us such a property.

**Lemma 2.1.16.** The positive cone  $L_1(\Omega, \mu)_+$  is a weakly closed subset of  $L_1(\Omega, \mu)$ .

*Proof.* Let  $\{f_n\} \subset L_1(\Omega, \mu)_+$  be such  $f_n \rightharpoonup f$  in  $L_1(\Omega, \mu)$ . We may then write

$$\begin{aligned} 0 &\geq \int_{\Omega} f \chi_{\{x:f<0\}} \, d\mu \\ &= \int_{\Omega} (f - f_n) \chi_{\{x:f<0\}} \, d\mu + \underbrace{\int_{\Omega} f_n \chi_{\{x:f<0\}} \, d\mu}_{\geq 0} \\ &\geq \int_{\Omega} (f - f_n) \chi_{\{x:f<0\}} \, d\mu. \end{aligned}$$

By Hölder's inequality,  $f \mapsto \int_{\Omega} f \chi_{\{x:f<0\}} \, d\mu$  defines a bounded linear functional on  $L_1(\Omega, \mu)$ . Hence if we let  $n \rightarrow \infty$ , the weak convergence of  $\{f_n\}$  gives us

$$0 \geq \int_{\Omega} f \chi_{\{x:f<0\}} \, d\mu \geq 0 \Rightarrow \int_{\{x:f<0\}} f \, d\mu = 0.$$

From this we may deduce that the set on which  $f$  takes negative values must have zero  $\mu$ -measure, therefore  $f \in L_1(\Omega, \mu)_+$ . That is  $L_1(\Omega, \mu)_+$  is a weakly closed subset.  $\square$

The main part of our convergence argument utilises the Dunford–Pettis theorem, which provides us with sufficient conditions to establish the weak convergence of our sequence of approximations. One such condition is that of *equiintegrability* which we introduce below.

**Definition 2.1.17.** Let  $(\Omega, \mathcal{A}, \mu)$  be a measure space. A family  $\mathcal{F}$  of measurable functions  $u : \Omega \rightarrow [-\infty, \infty]$  is said to be *equiintegrable* (uniformly integrable) if for every  $\varepsilon > 0$  there exists a  $\delta > 0$  such that

$$\sup_{f \in \mathcal{F}} \int_A |f| \, d\mu \leq \varepsilon,$$

for every measurable set  $A \subset \Omega$  with  $\mu(A) \leq \delta$ .

Essentially this condition says that integrals over sets of small measure are uniformly small. In our application setting this will ensure that the mass of the system does not become too concentrated. There are a number of equivalent characterisations of equiintegrability, which the reader may find in [32, Theorem 2.29]. For our purposes the most important characterisation of equiintegrability is given by de la Vallée Poussin's theorem, a refined version of which is given below.

**Theorem 2.1.18.** (de la Vallée Poussin's Theorem) *Let  $\mathcal{F}$  be a bounded subset of  $L_1(\Omega, \mu)$ , then  $\mathcal{F}$  is equiintegrable if and only if there exists a non-negative, convex function  $\Phi \in C^\infty([0, \infty))$ , with  $\Phi(0) = 0$  and  $\Phi'(0) = 1$ , such that  $\Phi'$  is concave and*

$$\frac{\Phi(x)}{x} \rightarrow \infty \text{ as } x \rightarrow \infty \text{ and } \sup_{f \in \mathcal{F}} \int_{\Omega} \Phi(|f|) \, d\mu < \infty.$$

*Proof.* The necessity of this condition can be derived easily from [51, Theorem 8], which under the assumption that  $\mathcal{F}$  is equiintegrable provides us with a  $\Psi$  satisfying all the stated conditions with the exception that the function  $\Psi$  has derivative 0 at 0 and is not stated to be non-negative. Given such a  $\Psi$ , we set  $\Phi(x) = \Psi(x) + x$ . Then  $\Phi$  retains the required properties of  $\Psi$  but additionally  $\Phi'(0) = 1$ . Also, by utilising the following standard inequality for  $C^1$  convex functions

$$\Phi(x) \geq \Phi(y) + \Phi'(y)(x - y), \quad (2.3)$$

with  $x \geq 0$  and  $y = 0$  we can see that  $\Phi(x)$  must be non-negative on  $[0, \infty)$ . The sufficiency of our conditions comes straight from the standard version of the de la Vallée Poussin theorem [32, Theorem 2.29 (iii)].  $\square$

In our analysis we shall require some properties of such a function, which we set out in the following lemma.

**Lemma 2.1.19.** *Let  $\Phi$  be as in Theorem 2.1.18; then for non-negative  $x$  and  $y$  we have the following:*

- (i)  $x\Phi'(y) \leq \Phi(x) + \Phi(y)$ ;
- (ii)  $\Phi'(y) \geq 0$ .

*Proof.* The first of these inequalities is non-standard and the proof can be found in [51, Proposition 13 (30)]. For the second property we return to inequality (2.3), with  $x = 0$  and  $y \geq 0$ , which gives us

$$\underbrace{\Phi(0)}_{=0} \geq \underbrace{\Phi(y)}_{\geq 0} + \Phi'(y)(0 - y).$$

An obvious rearrangement yields

$$y\Phi'(y) \geq \Phi(y) \geq 0.$$

Now in the case that  $y = 0$  property (ii) is given by the definition of  $\Phi$ . Hence we may assume that  $y > 0$  and divide through by it to obtain the desired result that  $\Phi'(y) \geq 0$ .  $\square$

We now come to the Dunford–Pettis theorem, one of the most significant technical tools applied in this work. The theorem provides necessary and sufficient conditions for a subset of an  $L_1$  space to be *weakly sequentially compact*. That is, any sequence in the subset must have a subsequence which is weakly convergent.

**Theorem 2.1.20.** (Dunford–Pettis Theorem) *Let  $(\Omega, \mathcal{A}, \mu)$  be a measure space and let  $\mathcal{F} \subset L_1(\Omega, \mu)$ . Then  $\mathcal{F}$  is weakly sequentially compact if and only if the following conditions are satisfied:*

- (i)  $\mathcal{F}$  is bounded in  $L_1(\Omega, \mu)$ ;

(ii)  $\mathcal{F}$  is equiintegrable;

(iii) For every  $\varepsilon > 0$  there exists  $A_\varepsilon \subset \Omega$  with  $A_\varepsilon \in \mathcal{A}$  such that  $\mu(A_\varepsilon) < \infty$  and

$$\sup_{f \in \mathcal{F}} \int_{\Omega \setminus A_\varepsilon} |f| \, d\mu \leq \varepsilon.$$

We note that in the case that  $\mu(\Omega) < \infty$  condition (iii) is automatically satisfied by taking  $A_\varepsilon = \Omega$  for all values of  $\varepsilon$ .

*Proof.* See [32, Theorem 2.54]. □

## 2.2 Calculus of Vector-Valued Functions

In this section we shall consider functions which map from an interval  $I$  in  $\mathbb{R}$  into a normed vector space  $(X, \|\cdot\|)$ . We will generalise a number of concepts from standard calculus of real-valued functions. This generally involves the simple substitution of the relevant norm in place of the modulus in the standard definitions.

**Definition 2.2.1.** The function  $f : I \rightarrow X$  is said to be *strongly continuous at the point*  $c \in I$ , if for each  $\varepsilon > 0$ , there exists a  $\delta > 0$  such that

$$\|f(t) - f(c)\| < \varepsilon \text{ whenever } t \in I \text{ and } |t - c| < \delta. \quad (2.4)$$

- The function  $f$  is said to be *strongly continuous on the interval*  $I$ , if  $f$  is strongly continuous at all points  $c \in I$ ;
- The set of all functions  $f : I \rightarrow X$ , which are continuous on  $I$  is denoted by  $C(I, X)$ ;
- If for all  $\varepsilon$  we can find a  $\delta$ , such that (2.4) holds for all  $c \in I$ , then we say that  $f$  is (strongly) *uniformly continuous* on  $I$ ;
- In the case of  $X$  being a Banach space and  $I = [\alpha, \beta]$  with  $-\infty < \alpha < \beta < \infty$ , then  $C([\alpha, \beta], X)$  forms a Banach space under the norm

$$\|f\|_\infty = \sup \{\|f(t)\|, t \in [\alpha, \beta]\};$$

see [14, Theorem 1.39].

**Definition 2.2.2.** The function  $f : I \rightarrow X$  is said to be *strongly differentiable at the point*  $c \in I$ , if there exists some element  $g \in X$  such that, for all  $\varepsilon > 0$ , we can find a corresponding  $\delta > 0$  such that

$$\left\| \frac{f(c+h) - f(c)}{h} - g \right\| < \varepsilon \text{ whenever } c+h \in I \text{ and } 0 < |h| < \delta.$$

The element  $g$  is referred to as the *strong derivative* of  $f$  at  $c$ , and is often denoted by  $f'(c)$ .

- A function  $f$  that is (strongly) differentiable at a point is necessarily (strongly) continuous at that point;
- If the function  $f$  is strongly differentiable at all points  $c \in I$ , then we say that  $f$  is *strongly differentiable on  $I$* ;
- Suppose that  $f$  is differentiable on  $I$  and that the derivative  $f'$  is continuous on  $I$ , then we say that  $f$  is *strongly continuously differentiable on  $I$* . The set of all such functions is denoted by  $C^1(I, X)$ .

Having defined a notion of differentiability, we now define two approaches to vector-valued integration and outline a number of key results concerning these constructs.

**Definition 2.2.3.** Suppose that  $f : [\alpha, \beta] \rightarrow X$  where  $-\infty < \alpha < \beta < \infty$ . Let us denote by  $P_n$  the following partition of the interval  $[\alpha, \beta]$ :

$$P_n : \alpha = t_0 < t_1 < t_2 < \cdots < t_n = \beta,$$

and introduce the following ‘measure’ of this partition:

$$\|P_n\| = \max_{1 \leq m \leq n} (t_m - t_{m-1}).$$

As we would with a real-valued function, we can form a Riemann sum of  $f$  over this partition, defined by

$$S(f; P_n) = \sum_{m=1}^n f(\overline{t_m})(t_m - t_{m-1}),$$

where  $\overline{t_m}$  is an arbitrary point from  $[t_{m-1}, t_m]$ . If we consider a sequence of such Riemann sums and find that they converge in  $X$  as  $\|P_n\| \rightarrow 0$ , and if the limit is independent of the manner in which  $\|P_n\| \rightarrow 0$ , then we say that  $f$  is *Riemann integrable* on  $[\alpha, \beta]$ . We denote the common limit by  $\int_{\alpha}^{\beta} f(t) dt$  and refer to it as the *strong Riemann integral* of  $f$  over  $[\alpha, \beta]$ .

Checking whether a function is integrable in this way may be rather involved in practice. However, as with real-valued integration, certain classes of functions can be shown to be automatically Riemann integrable. In the following theorem we cover an important class of integrable functions, before going on to detail a number of important properties and results concerning their integrals.

**Theorem 2.2.4.** *Let  $X$  be a real Banach space and let  $f : [\alpha, \beta] \rightarrow X$  be strongly continuous. Then  $f$  is Riemann integrable on  $[\alpha, \beta]$ .*

*Proof.* See [14, Theorem 1.43]. □

**Theorem 2.2.5.** *Let  $X$  be a real Banach space and let  $f : [\alpha, \beta] \rightarrow X$  be strongly continuous. Then by the previous result  $f$  is Riemann integrable and its integral satisfies*

$$\left\| \int_{\alpha}^{\beta} f(t) dt \right\| \leq \int_{\alpha}^{\beta} \|f(t)\| dt,$$

where the right-hand integral is a standard real-valued Riemann integral.

*Proof.* See [14, Theorem 1.44]. □

Improper integrals on infinite or semi-infinite intervals can be tackled in the same manner as we would handle real-valued integrals. For example, suppose  $f : [\alpha, \infty) \rightarrow X$ , then we may consider defining  $\int_{\alpha}^{\infty} f(t) dt$  as follows:

$$\int_{\alpha}^{\infty} f(t) dt = \lim_{\tau \rightarrow \infty} \int_{\alpha}^{\tau} f(t) dt, \quad \text{if this limit exists.}$$

The following theorem provides a condition under which such a limit will exist.

**Theorem 2.2.6.** *Let  $X$  be a real Banach space and let  $f : [\alpha, \infty) \rightarrow X$  be strongly continuous. If the real integral  $\int_{\alpha}^{\infty} \|f(t)\| dt$  exists, then  $\int_{\alpha}^{\infty} f(t) dt$  exists in  $X$  and we have*

$$\left\| \int_{\alpha}^{\infty} f(t) dt \right\| \leq \int_{\alpha}^{\infty} \|f(t)\| dt.$$

*Proof.* See [14, Theorem 1.45]. □

**Theorem 2.2.7.** (Fundamental Theorem of Calculus) *Let  $X$  be a real Banach space and let  $f : [\alpha, \beta] \rightarrow X$  be strongly continuous. Then, for each  $t \in [\alpha, \beta]$ , the integral  $\int_{\alpha}^t f(s) ds$  exists in  $X$  and*

$$\frac{d}{dt} \int_{\alpha}^t f(s) ds = f(t).$$

If  $f$  is additionally  $C^1$  on  $(\alpha, \beta)$ , then

$$\int_{\alpha}^{\beta} f'(s) ds = f(\beta) - f(\alpha),$$

whenever the right-hand side is defined (in particular when  $f'$  can be continuously extended to  $[\alpha, \beta]$ ).

*Proof.* See [47, Page 340] and [35, Theorem 89]. □

As with integration of real-valued functions, the Riemann integral can prove insufficient for our needs and so we may consider introducing alternative forms of integral. One such approach is the Bochner integral, which we now introduce. The Bochner integral extends Lebesgue integration to Banach space valued functions. In what follows let  $I \subset \mathbb{R}$  be some interval, let  $\lambda$  denote the Lebesgue measure and let  $(X, \|\cdot\|)$  be a Banach space.

**Definition 2.2.8.** An  $X$ -valued function  $s : I \rightarrow X$  is called a *simple function* if it can be represented in the form

$$s = \sum_{k=1}^n x_k \chi_{I_k},$$

for elements  $x_k \in X$  and disjoint measurable sets  $I_k \subset I$ . We say that such a function is *Bochner integrable* if  $x_k = 0$  whenever  $\lambda(I_k) = \infty$ , and define its (Bochner) integral to be

$$\int_I s(t) dt = \sum_{k=1}^n x_k \lambda(I_k).$$

**Definition 2.2.9.** If the function  $f : I \rightarrow X$  (defined almost everywhere on  $I$ ) can be approximated pointwise on  $I$  by simple functions, that is if there exists a sequence  $\{s_n\}_{n \in \mathbb{N}}$  of simple functions on  $I$  such that

$$\lim_{n \rightarrow \infty} \|f(t) - s_n(t)\| = 0 \quad \text{for almost all } t \in I,$$

then we call  $f$  (*Bochner*) *measurable*. If  $f$  is measurable and there exists a sequence  $\{s_n\}_{n \in \mathbb{N}}$  of simple functions on  $I$  such that

$$\lim_{n \rightarrow \infty} \int_I \|f(t) - s_n(t)\| dt = 0,$$

then we say that  $f$  is *Bochner integrable*. For such an  $f$  its *Bochner integral* is defined by

$$\int_I f(t) dt = \lim_{n \rightarrow \infty} \int_I s_n(t) dt.$$

The above definition of integrability may prove unwieldy to use in practice. The following result provides a more applicable characterisation which we shall make use of in our analysis.

**Theorem 2.2.10.** *The measurable function  $f : I \rightarrow X$  is integrable if and only if*

$$\int_I \|f(t)\| dt < \infty,$$

*in which case we have*

$$\left\| \int_I f(t) dt \right\| \leq \int_I \|f(t)\| dt.$$

*Proof.* See [24, Chapter 2, Theorem 2 and Theorem 4]. □

*Remark 2.2.11.* The Bochner integral provides many of the familiar results from scalar valued integration such as Fubini's theorem and Lebesgue's dominated convergence theorem. For a full account of the Bochner integral and its properties the reader is directed to [36, Chapter 3].

**Theorem 2.2.12.** *Let  $f : [\alpha, \beta] \rightarrow X$  be continuous; then the Riemann and Bochner integrals of  $f$  over  $[\alpha, \beta]$  both exist and agree.*

*Proof.* Let  ${}_R \int$  and  ${}_B \int$  denote the Riemann and Bochner integrals respectively. Let  $P_n$  denote a partition of  $[\alpha, \beta]$  as in Definition 2.2.3 and let  $\tau_k = [t_{k-1}, t_k]$  for  $k = 1, \dots, n-1$ , and  $\tau_n = [t_{n-1}, t_n]$ , so that  $\|P_n\| \rightarrow 0$  as  $n \rightarrow \infty$ . By Theorem 2.1.20,  $f$  is Riemann integrable and

$${}_R \int_{\alpha}^{\beta} f(t) dt = \lim_{\|P_n\| \rightarrow 0} S(f; P_n) = \lim_{n \rightarrow \infty} \sum_{k=1}^n f(\bar{t}_k) \lambda(\tau_k),$$

where  $\bar{t}_k$  is any point in  $\tau_k$  and  $\lambda$  is the Lebesgue measure. Given such a sequence of partitions we define the simple functions  $s_n : [\alpha, \beta] \rightarrow X$  by

$$s_n(t) = \sum_{k=1}^n \chi_{\tau_k}(t) f(\bar{t}_k).$$

Using the properties of a norm we then have

$$\begin{aligned} \|f(t) - s_n(t)\| &= \left\| f(t) - \sum_{k=1}^n \chi_{\tau_k}(t) f(\bar{t}_k) \right\| \\ &= \left\| \sum_{k=1}^n \chi_{\tau_k}(t) (f(t) - f(\bar{t}_k)) \right\| \\ &\leq \sum_{k=1}^n \chi_{\tau_k}(t) \|f(t) - f(\bar{t}_k)\|. \end{aligned} \quad (2.5)$$

Let us fix  $t \in [\alpha, \beta]$ ; then, by the continuity of  $f$ , given  $\varepsilon > 0$  we can find  $\delta > 0$  such that

$$\|f(t') - f(t)\| < \varepsilon \text{ for all } t' \in [\alpha, \beta], \text{ such that } |t' - t| < \delta.$$

Let us now take  $N$  such that  $\|P_n\| < \delta$  for all  $n \geq N$ . For all such  $n$ , our fixed  $t$  must belong to exactly one of the intervals  $\tau_k$ , say  $t \in \tau_{m(n)}$ . Then we have  $|\bar{t}_{m(n)} - t| < \delta$  so that  $\|f(\bar{t}_{m(n)}) - f(t)\| < \varepsilon$ . The inequality (2.5) then becomes

$$\|f(t) - s_n(t)\| \leq \|f(\bar{t}_{m(n)}) - f(t)\| < \varepsilon, \text{ for all } n \geq N.$$

Therefore we have for each  $t \in [\alpha, \beta]$  that

$$\lim_{n \rightarrow \infty} \|f(t) - s_n(t)\| = 0, \quad (2.6)$$

hence  $f$  is measurable. As the norm  $\|\cdot\| : X \rightarrow \mathbb{R}$  is continuous,  $\|f(\cdot)\| : [\alpha, \beta] \rightarrow \mathbb{R}$  defines a continuous mapping hence it is bounded on finite closed intervals.

Therefore there exists an  $M \in \mathbb{R}$  such that  $\|f(t)\| \leq M$ , for all  $t \in [\alpha, \beta]$ . As each  $t \in [\alpha, \beta]$  belongs to exactly one  $\tau_k$ , we have

$$\|s_n(t)\| \leq \sum_{k=1}^n \chi_{\tau_k}(t) \|f(\bar{t}_k)\| \leq M,$$

and therefore, for all  $t \in [\alpha, \beta]$  the following bound holds

$$\|f(t) - s_n(t)\| \leq \|f(t)\| + \|s_n(t)\| \leq 2M.$$

This, along with (2.6), allows us to apply the scalar version of Lebesgue's dominated convergence theorem to get

$$\lim_{n \rightarrow \infty} \int_{\alpha}^{\beta} \|f(t) - s_n(t)\| \, ds = \int_{\alpha}^{\beta} \lim_{n \rightarrow \infty} \|f(t) - s_n(t)\| \, ds = 0.$$

Hence  $f$  is Bochner integrable and its integral is given by

$${}_B \int_{\alpha}^{\beta} f(t) \, dt := \lim_{n \rightarrow \infty} \int_{\alpha}^{\beta} s_n(t) \, ds = \lim_{n \rightarrow \infty} \sum_{k=1}^n f(\bar{t}_k) \lambda(\tau_k) =_R \int_{\alpha}^{\beta} f(t) \, dt.$$

□

This result allows us to ascertain that the results of Theorem 2.4.15 and Theorem 2.4.15 hold for the Bochner integral.

**Definition 2.2.13.** As was the case with scalar-valued functions, if we consider the classes of functions  $f : I \rightarrow X$  which differ only on sets of Lebesgue measure zero, then the spaces  $(L_p(I, X), \|\cdot\|_p)$  defined by

$$L_p(I, X) := \left\{ f : I \rightarrow X : f \text{ is measurable, and } \|f\|_p^p := \int_I \|f(t)\|^p \, dt < \infty \right\},$$

for  $1 \leq p < \infty$  and

$$L_{\infty}(I, X) := \left\{ f : I \rightarrow X : f \text{ is measurable, and } \|f\|_{\infty} := \operatorname{ess\,sup}_{s \in I} \|f(s)\| < \infty \right\},$$

form Banach spaces.

*Proof.* See [26, Chapter 3, Theorem 6.6]. □

For our applications we will be considering the case  $p = 1$  with  $X = L_1(\Omega, d\mu)$ , and we now examine the relationship between  $L_1(I, L_1(\Omega, d\mu))$  and  $L_1(I \times \Omega, dt \, d\mu)$ .

Going from  $L_1(I \times \Omega, dt \, d\mu)$  to  $L_1(I, L_1(\Omega, d\mu))$  is rather straightforward; for any  $f \in L_1(I \times \Omega, dt \, d\mu)$ , the Fubini theorem tells us that  $f$  is  $\mu$ -integrable over

$\Omega$  for almost all  $t \in I$ , hence can be treated as an element of  $L_1(I, L_1(\Omega, d\mu))$ .

However the space  $L_1(I, L_1(\Omega, d\mu))$  does in fact consist of equivalence classes of equivalence classes of functions. Given some  $f \in L_1(I, L_1(\Omega, d\mu))$ , for each  $t \in I$ ,  $f(t)$  is an equivalence class of functions, such that any pair of members agree  $\mu$ -almost everywhere. If we select a particular  $\bar{f}(t, \cdot) \in f(t)$ , then the resulting function  $\bar{f}(t, x)$  defined on the product  $I \times \Omega$  is called a *representative* of  $f$ . It is not immediately clear whether we can define a representation  $\bar{f}(t, x)$ , measurable on  $I \times \Omega$ , such that for almost all  $(t, x) \in I \times \Omega$ . This question is answered in the affirmative in the following theorems along with further shared properties of abstract Banach space valued functions and their measurable representations.

**Theorem 2.2.14.** *Let  $0 < T \leq \infty$  and let  $(\Omega, \mathcal{A}, \mu)$  be a positive measure space. Let us denote by  $dt$  the Lebesgue measure on  $[0, T)$ .*

- (i) *If  $f : [0, T) \rightarrow L_1(\Omega, d\mu)$  is a (Bochner) integrable function on  $[0, T)$ , then there exists an integrable function  $\bar{f} : [0, T) \times \Omega \rightarrow \mathbb{R}$ , such that  $\bar{f}(t, \cdot) = f(t)$  for almost all  $t \in [0, T)$ . Furthermore this  $\bar{f}$  is uniquely determined except on a set of (product) measure zero;*
- (ii) *Conversely, suppose  $\bar{f} : [0, T) \times \Omega \rightarrow \mathbb{R}$  is integrable. Then the function  $f : [0, T) \rightarrow L_1(\Omega, d\mu)$  defined for almost all  $t \in [0, T)$  by  $f(t) := \bar{f}(t, \cdot)$  is integrable.*

Further, in both of these cases we have

$$\left[ \int_0^T f(t) dt \right] (\cdot) = \int_0^T \bar{f}(t, \cdot) dt,$$

which holds on almost all of  $\Omega$ , where the left-hand integral above is the Bochner integral and the right-hand integral is usual Lebesgue integral of a scalar-valued function.

*Proof.* See [26, Theorem 3.11.14 and Corollary 3.11.15 (page 194) and Theorem 3.11.17 (page 198)]. □

**Theorem 2.2.15.** *Suppose that  $f : [0, T) \rightarrow L_1(\Omega, d\mu)$  is  $n$ -times continuously differentiable, in the sense of Definition 2.2.2. Then there exists a real-valued function  $\bar{f}(t, x)$ , measurable on  $[0, T) \times \Omega$ , such that for almost all  $x \in \Omega$  and  $0 \leq k \leq n - 1$ ,  $\partial_t^k \bar{f}(t, x)$  is absolutely continuous w.r.t.  $t$  and  $\partial_t^k \bar{f}(t, \cdot) = f^{(k)}(t)$  for a.a.  $t \in [0, T)$ . Moreover  $\partial_t^n \bar{f}(t, x)$  exists almost everywhere in  $[0, T) \times \Omega$  and  $\partial_t^n \bar{f}(t, \cdot) = f^{(n)}(t)$  for almost all  $t \in [0, T)$ . Further, by Theorem 2.2.14(i) this numerical representation is unique up to a set of measure zero.*

*Proof.* See [10, Theorem 2.40]. □

These results allow us to treat the two spaces as essentially identical for our purposes and to switch between them when mathematically convenient.

## 2.3 Operators

We now consider operators which map from one normed vector space to another. In terms of background knowledge, we assume a familiarity with basic concepts such as linearity and boundedness, but in this section we provide an overview of the required concepts relating to operators which may be considered less standard.

In what follows we shall assume  $(X, \|\cdot\|)$ ,  $(X_1, \|\cdot\|_{X_1})$  and  $(X_2, \|\cdot\|_{X_2})$  to be (real) normed vector spaces, unless otherwise stated.

**Definition 2.3.1.** The operator  $A : D(A) \subseteq X_1 \rightarrow X_2$  is said to be *closed* if whenever a sequence  $\{f_n\}_{n=1}^\infty \subset D(A)$  is such that  $f_n \rightarrow f$  in  $X_1$  and  $Af_n \rightarrow g$  in  $X_2$ , then  $f \in D(A)$  and  $Af = g$ .

**Definition 2.3.2.** The *graph* of the operator  $A : D(A) \subseteq X_1 \rightarrow X_2$  is the subset  $G(A)$  of  $(X_1 \times X_2, \|\cdot\|_{X_1 \times X_2})$  defined by

$$G(A) = \{(f, g) : f \in D(A), g = Af\}.$$

**Lemma 2.3.3.** *The operator  $A : D(A) \subseteq X_1 \rightarrow X_2$  is closed if and only if its graph  $G(A)$  is a closed subset of  $(X_1 \times X_2, \|\cdot\|_{X_1 \times X_2})$ .*

*Proof.* See [14, Theorem 1.64]. □

**Lemma 2.3.4.** *Let  $X$  be a Banach space and let  $A : D(A) \subseteq X \rightarrow X$  be a closed operator. Suppose that  $f : I \rightarrow X$  is Bochner integrable, where  $I$  denotes some interval. If  $f$  is such that  $f(t) \in D(A)$  for all  $t \in I$  and  $Af : I \rightarrow X$  is Bochner integrable, then  $\int_I f(t) dt \in D(A)$  and*

$$A \int_I f(t) dt = \int_I A(f(t)) dt.$$

*For  $A \in B(X)$  the above holds for any  $f : I \rightarrow X$  which is Bochner integrable, the additional requirements being satisfied automatically.*

*Proof.* See [4, Proposition 1.1.7.]. □

**Definition 2.3.5.** Let  $A : D(A) \subseteq X_1 \rightarrow X_2$ . A sequence  $\{f_n\}_{n=1}^\infty \subset D(A)$  is said to be *A-convergent* to  $f \in X_1$ , if  $\{f_n\}_{n=1}^\infty$  converges in  $X_1$  to  $f$  and  $\{Af_n\}_{n=1}^\infty$  is a Cauchy sequence in  $X_2$ .

**Definition 2.3.6.** Let  $A : D(A) \subseteq X_1 \rightarrow X_2$  and  $A' : D(A') \subseteq X_1 \rightarrow X_2$ . We say that  $A'$  is an *extension* of  $A$  if  $D(A) \subseteq D(A')$  and  $A'f = Af$  for all  $f \in D(A)$ . The case that  $D(A) = D(A')$  and  $A \equiv A'$  is trivial and typically when we refer to an extension we expect to have  $D(A) \subset D(A')$ .

**Definition 2.3.7.** Let  $(X_1, \|\cdot\|_1)$  and  $(X_2, \|\cdot\|_2)$  be two Banach spaces. We say that the linear operator  $A : D(A) \subseteq X_1 \rightarrow X_2$  is *closable* if it has a closed extension. Given a closable operator  $A$ , we call its smallest closed extension the *closure* of  $A$ , which we denote by  $\overline{A}$ . An element  $f \in X_1$  belongs to  $D(\overline{A})$  if and only if there exists a sequence  $\{f_n\}_{n=1}^\infty$  in  $D(A)$  which is  $A$ -convergent to  $f$ . In this case  $\overline{A}f = \lim_{n \rightarrow \infty} Af_n$ ; see [40, page 166].

**Definition 2.3.8.** Suppose that  $(X_1, \|\cdot\|_1)$  and  $(X_2, \|\cdot\|_2)$  are real Banach spaces equipped with positive cones  $X_{1+}$  and  $X_{2+}$ , respectively. We say that the operator  $A : D(A) \subseteq X_1 \rightarrow X_2$  is *positive* if it maps  $D(A)_+ = D(A) \cap X_{1+}$  into  $X_{2+}$ .

**Definition 2.3.9.** Let  $X$  be a Banach space and  $A : D(A) \subseteq X \rightarrow X$  a linear operator. Then the *resolvent set*,  $\rho(A)$ , of  $A$  is defined by

$$\rho(A) = \{\lambda \in \mathbb{C} : (\lambda I - A)^{-1} \in B(X)\}.$$

For  $\lambda \in \rho(A)$  the operator given by

$$R(\lambda, A) = (\lambda I - A)^{-1},$$

is called the *resolvent operator* of  $A$ . The *spectrum* of  $A$ , denoted  $\sigma(A)$ , is defined as the complement of the resolvent set,  $\rho(A)$ , in  $\mathbb{C}$ , that is

$$\sigma(A) = \mathbb{C} \setminus \rho(A) = \{\lambda \in \mathbb{C} : \lambda \notin \rho(A)\}.$$

**Definition 2.3.10.** Let  $(X_1, \|\cdot\|_1)$  and  $(X_2, \|\cdot\|_2)$  be Banach spaces and let  $A : D(A) \subseteq X_1 \rightarrow X_1$  and  $B : D(B) \subseteq X_1 \rightarrow X_2$  be operators with  $D(A) \subseteq D(B)$ . We say that  $B$  is *A-bounded* (or  $B$  is *relatively A-bounded*) if there exist non-negative constants  $a$  and  $b$  such that

$$\|Bf\|_2 \leq a\|Af\|_1 + b\|f\|_1 \text{ for all } f \in D(A). \quad (2.7)$$

The infimum of the values of  $a$  for which such a bound exists is known as the *A-bound* of  $B$ .

**Lemma 2.3.11.** *Let  $(X_1, \|\cdot\|_1)$  and  $(X_2, \|\cdot\|_2)$  be Banach spaces and let the operators  $A : D(A) \subseteq X_1 \rightarrow X_1$  and  $B : D(B) \subseteq X_1 \rightarrow X_2$  be linear, with  $D(A) \subseteq D(B)$  and  $\rho(A) \neq \emptyset$ . Then  $B$  is  $A$ -bounded if and only if  $BR(\lambda, A) \in B(X_1, X_2)$  for some  $\lambda \in \rho(A)$ .*

This is a more general version of the result given in [10, Lemma 4.1]. Therefore, for completeness we include the following proof of the lemma.

*Proof.* Let the operator  $B$  be  $A$ -bounded and let  $g \in X_1$ . Then for  $\lambda \in \rho(A)$  we have  $R(\lambda, A)g \in D(A)$  and there exist non-negative constants  $a$  and  $b$ , such that

$$\|BR(\lambda, A)g\|_2 \leq a\|AR(\lambda, A)g\|_1 + b\|R(\lambda, A)g\|_1.$$

Rewriting  $AR(\lambda, A)g$ , as follows:

$$AR(\lambda, A)g = (A - \lambda I)R(\lambda, A)g + \lambda R(\lambda, A)g = \lambda R(\lambda, A)g - g,$$

the previous inequality becomes

$$\begin{aligned} \|BR(\lambda, A)g\|_2 &\leq a\|\lambda R(\lambda, A)g - g\|_1 + b\|R(\lambda, A)g\|_1 \\ &\leq (a|\lambda| + b)\|R(\lambda, A)g\|_1 + a\|g\|_1. \end{aligned}$$

As  $\lambda \in \rho(A)$ , there exists a constant  $M \geq 0$  such that  $\|R(\lambda, A)g\|_1 \leq M\|g\|_1$ , for any  $g \in X_1$ . Therefore

$$\|BR(\lambda, A)g\|_2 \leq (Ma|\lambda| + Mb + a)\|g\|_1.$$

Hence  $BR(\lambda, A) \in B(X_1, X_2)$ . Now conversely, suppose that  $BR(\lambda, A) \in B(X_1, X_2)$  for some  $\lambda \in \rho(A)$ , with  $\|BR(\lambda, A)\| = K$ . If  $f \in D(A)$ , then  $f = R(\lambda, A)g$  for some  $g \in X_1$ . Therefore

$$\|Bf\|_2 = \|BR(\lambda, A)g\|_2 \leq K\|g\|_1 = K\|(\lambda I - A)f\|_1 \leq K\|Af\|_1 + |\lambda|K\|f\|_1.$$

Hence  $B$  is  $A$ -bounded, as defined in Definition 2.3.10, completing the proof of the result.  $\square$

**Lemma 2.3.12.** *Let  $X$  be a Banach space and let  $A : D(A) \subseteq X \rightarrow X$  be closed, and  $B : D(B) \subseteq X \rightarrow X$  be  $A$ -bounded with  $A$ -bound strictly less than 1. Then the sum  $(A + B, D(A))$  is a closed operator.*

*Proof.* See [28, Chapter 3, Lemma 2.4].  $\square$

**Definition 2.3.13.** A subspace  $D$  of the domain  $D(A)$  of a linear operator  $A : D(A) \subseteq X \rightarrow X$  is called a *core* for the operator  $A$ , if  $D$  is dense in  $D(A)$  for the graph norm

$$\|f\|_A = \|f\| + \|Af\|.$$

**Definition 2.3.14.** If  $(A, D(A))$  is an operator in  $X$  and  $Y \subset X$ , then the *part* of  $A$  in  $Y$ , denoted  $A_Y$ , is defined by

$$A_Y f = Af, \text{ on the domain } D(A_Y) = \{f \in D(A) \cap Y : Af \in Y\}.$$

The *restriction* of  $(A, D(A))$  to  $D \subset D(A)$  is denoted by  $A|_D$  and defined simply as

$$A|_D f = Af, \text{ for } f \in D.$$

## 2.4 Semigroups

For much of the analysis in this thesis we shall be relying on the tools provided by the theory of semigroups. This section provides an introduction to the concept of an operator semigroup and gives an account of the key results in this area. We conclude the section by indicating how the theory can be used to tackle problems of the type we shall be considering.

### 2.4.1 Introduction to Semigroups

As a way of motivating what follows, let us imagine a dynamical system evolving with time. Supposing that the state of the system can be represented as an element of some Banach space  $X$ , so that at each point in time  $t$  the system is described by  $u(t) \in X$ . The evolution of the system can then be thought of as defining a family of transition operators  $(T(s))_{s \geq 0}$ , whereby applying  $T(s)$  has the effect of advancing the system state through a time interval of length  $s$ . If the initial state of the system were described by  $u_0 = u(0)$ , then the state at a subsequent time  $t \geq 0$  would be given by

$$u(t) = T(t)u_0, \quad (t \geq 0).$$

Let us now consider some of the properties that the operators  $(T(s))_{s \geq 0}$  should possess. Since no transition can take place over a time interval of zero length, we would expect the application of  $T(0)$  to leave the system state unchanged. Therefore we should have  $T(0) = I_X$ , where  $I_X$  is the identity operator on  $X$ . Additionally, if the system evolved for an initial period of length  $t$ , before evolving for a further period of length  $s$ , then we would expect to find it in the same state as we would had it simply evolved over an interval of length  $s+t$ . We should therefore expect the operators  $(T(s))_{s \geq 0}$  to satisfy  $T(s+t) = T(s)T(t)$  for all  $s, t \geq 0$ . This concept of a family of evolution operators is formalised in the following section, before we go on to develop the theory surrounding such a family.

### 2.4.2 Strongly Continuous Semigroups

**Definition 2.4.1.** Let  $X$  be a Banach space. Then a family of operators  $(T(t))_{t \geq 0} \subset B(X)$  forms a  $C_0$ -semigroup (*strongly continuous semigroup*) of operators on  $X$ , if it satisfies the following conditions:

- (i)  $T(0) = I_X$  where  $I_X$  is the identity operator on  $X$ ;
- (ii)  $T(s+t) = T(s)T(t)$  for all  $s, t \geq 0$ ;
- (iii)  $\|T(t)f - f\|_X \rightarrow 0$  as  $t \rightarrow 0^+$  for any fixed  $f \in X$ .

Conditions (i) and (ii) are motivated by the previous consideration of a system evolving with time. It is common to see condition (ii) referred to as the *semigroup property* in the literature. The continuity condition (iii) might appear weak. However, in conjunction with conditions (i) and (ii) it can be used to establish further results. Having said this, perhaps a more obvious choice would be to replace (iii) with the following alternative:

$$\|T(t) - I\|_{B(X)} \rightarrow 0 \quad \text{as } t \rightarrow 0^+. \quad (2.8)$$

Replacing condition (iii) of Definition 2.4.1 with the above alternative provides us with a stricter class of semigroup, which is described in the following definition.

**Definition 2.4.2.** A family of operators  $(T(t))_{t \geq 0} \subset B(X)$  satisfying the conditions (i) and (ii) of Definition 2.4.1 and (2.8) is known as a *uniformly continuous semigroup*. This condition is stronger than (iii) above, with each uniformly continuous semigroup automatically forming a  $C_0$ -semigroup, whilst the converse is not, in general, true.

For many applications the condition (2.8) proves too strong and we will mainly be utilising strongly continuous semigroups and their properties.

**Theorem 2.4.3.** *Let  $X$  be a Banach space and  $(T(t))_{t \geq 0}$  a  $C_0$ -semigroup on  $X$ . Then there exist constants  $M \geq 1$  and  $\omega \in \mathbb{R}$  such that*

$$\|T(t)\| \leq Me^{\omega t} \quad \text{for } t \geq 0. \quad (2.9)$$

*The infimum of the values of  $\omega$  for which such a bound can be formed, is called the growth bound of the semigroup.*

*Proof.* See [28, Chapter 2, Theorem 1.10]. □

If we are able to form a bound of the form (2.8), where  $M = 1$  and  $\omega = 0$ , then we say that we have a semigroup of contractions or a contraction semigroup. For our purposes, an important class of such semigroups are *substochastic* semigroups, which we now introduce.

**Definition 2.4.4.** Let  $X$  denote a Banach space of the type  $L_1(\Omega, \mu)$  with positive cone  $X_+$ . Let  $(T(t))_{t \geq 0}$  be a  $C_0$ -semigroup on  $X$ . We say that  $(T(t))_{t \geq 0}$  is a *substochastic* semigroup on  $X$  if, for each  $t \geq 0$ ,  $\|T(t)\| \leq 1$  and  $T(t)f \in X_+$  for all  $f \in X_+$ . If additionally  $\|T(t)f\| = \|f\|$  for all  $t \geq 0$  when  $f \in X_+$ , then we say that  $(T(t))_{t \geq 0}$  is a *stochastic* semigroup.

**Lemma 2.4.5.** *Let  $X$  be a Banach space and let  $(T(t))_{t \geq 0}$  be a  $C_0$ -semigroup on  $X$ . Then, for each fixed  $f \in X$ , the mapping  $t \mapsto T(t)f$  is a continuous map from the non-negative real line into  $X$ .*

*Proof.* See [68, Chapter 1, Corollary 2.3]. □

### 2.4.3 Generators

Let us consider a complex scalar-valued function  $\phi : [0, \infty) \rightarrow \mathbb{C}$ , which satisfies the following properties:

- (i)  $\phi(0) = 1$ ;
- (ii)  $\phi(s + t) = \phi(s)\phi(t)$  for all  $s, t \geq 0$ ;
- (iii)  $\phi$  is continuous on  $[0, \infty)$ .

Then, as Cauchy proposed in [21], the function  $\phi$  must take the form  $e^{ta}$ , where  $a$  may be any complex constant. Comparing these conditions to those set out in Definition 2.4.1 together with Lemma 2.4.5, the resemblances are clear. Therefore, it is perhaps reasonable to think that given a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ , the operators would have the form  $T(t) = \exp(tA)$ , where  $A$  is some operator.

**Theorem 2.4.6.** *Let  $X$  be a Banach space and suppose that the power series  $\phi(z) = \sum_{n=0}^{\infty} a_n z^n$  has radius of convergence  $r > 0$ . Then for  $A \in B(X)$  such that  $\|A\| < r$ , the series*

$$\phi(A) = \sum_{n=0}^{\infty} a_n A^n, \quad (2.10)$$

*converges in  $B(X)$ , where  $A^n$  signifies composition of the operator  $A$  applied  $n$  times. Further, if the coefficients  $(a_0, a_1, a_2, \dots)$  are real and non-negative, then  $\|\phi(A)\| \leq \phi(\|A\|)$ .*

*Proof.* See [14, Theorem 1.86]. □

**Theorem 2.4.7.** *Recall that the exponential function  $\exp(z)$  has the power series representation  $\sum_{n=0}^{\infty} z^n/n!$  with infinite radius of convergence. Hence if  $A \in B(X)$ , then  $tA \in B(X)$  for each  $t \geq 0$ , and therefore*

$$\exp(tA) = \sum_{n=0}^{\infty} \frac{t^n A^n}{n!}, \quad (2.11)$$

*converges in  $B(X)$ . When  $A \in B(X)$ , then the family of operators  $(T(t))_{t \geq 0}$ , where  $T(t) = \exp(tA)$ , forms a uniformly continuous semigroup on  $X$ . In fact, it may be shown that every uniformly continuous semigroup on a Banach space takes this form for some  $A \in B(X)$ .*

*Proof.* See [28, Chapter 1, Theorem 3.7 and Chapter 2, Corollary 1.5]. □

Taking the series (2.11), and assuming it is valid to differentiate it term-by-term, we arrive at the following expression:

$$\frac{d}{dt} \{T(t)\} = A + \sum_{n=1}^{\infty} \frac{t^n A^{n+1}}{n!} \quad (t \geq 0).$$

When evaluated at  $t = 0$ , this gives

$$T'(0) = \left[ \frac{d}{dt} \{T(t)\} \right]_{t=0} = A.$$

Therefore, the operator  $A$  has been recovered from the semigroup by taking the (right) derivative of the semigroup, and evaluating it at  $t = 0$ . These operations have been carried out under the assumption that the operator  $A$  was bounded,

however this may not be the case in practice. We now look to extend the ideas outlined here to the case of a general  $C_0$ -semigroup. A significant concept in this task, and more widely in the theory of semigroups, is that of the *generator* of a semigroup, which is introduced below.

**Definition 2.4.8.** Let  $(T(t))_{t \geq 0}$  be a  $C_0$ -semigroup on a Banach space  $X$ . Then the (*infinitesimal*) *generator* of  $(T(t))_{t \geq 0}$  is the operator  $A : D(A) \subseteq X \rightarrow X$  defined as follows.

For  $t > 0$  and  $f \in X$ , let  $A_t f = \{T(t)f - f\} / t$ . Then

$$\left. \begin{aligned} D(A) &= \{f \in X : \lim_{t \rightarrow 0^+} A_t f \text{ exists in } X\} \\ A f &= \lim_{t \rightarrow 0^+} A_t f \text{ for } f \in D(A) \end{aligned} \right\}.$$

It is easily shown that the operator  $A$  is linear and that its domain  $D(A)$  is a vector subspace of  $X$ .

This general definition of the generator was guided by the approach adopted with the uniformly continuous semigroup, where we took the derivative of the semigroup and evaluated it at  $t = 0$ . However, in keeping with the continuity conditions of Definition 2.4.2 and Definition 2.4.1, we have moved from the space of bounded operators  $B(X)$ , to the Banach space  $X$ .

In the remainder of this section we will consider the idea of the generator further and establish some of its key properties. This will culminate in the most significant results concerning  $C_0$ -semigroups and their generators, namely the Hille–Yosida theorem and its generalisation. These theorems provide both necessary and sufficient conditions for an operator to generate a strongly continuous semigroup.

**Definition 2.4.9.** Let  $X$  be a Banach space. Then for real numbers  $M \geq 1$  and  $\omega \in \mathbb{R}$ , we denote by  $\mathcal{G}(M, \omega; X)$  the set of operators  $A$  which generate a  $C_0$ -semigroup on  $X$  that satisfies the bound (2.9). For the existence of such an  $M$  and  $\omega$ , see Theorem 2.4.3.

**Theorem 2.4.10.** (Rescaled Semigroups) *Let  $A$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ , which satisfies the bound (2.9). Then for any  $\mu \in \mathbb{R}$ ,  $(S(t))_{t \geq 0} := (e^{\mu t} T(t))_{t \geq 0}$  provides a  $C_0$ -semigroup which satisfies*

$$\|S(t)\| \leq M e^{(\omega + \mu)t} \text{ for } t \geq 0.$$

*The generator of this new semigroup is  $B = A + \mu I$ , with  $D(B) = D(A)$ .*

Although this result is stated in [28, page 60], no explanation is given and therefore we include the following proof.

*Proof.* It is easily shown that  $(S(t))_{t \geq 0}$ , as defined above, satisfies conditions (i)-(iii) from Definition 2.4.1. Firstly, evaluating at  $t = 0$ , we get

$$S(0) = e^{\mu 0} T(0) = e^0 I = I.$$

Confirming condition (i) holds. Secondly, for all  $s, t \geq 0$ , we obtain condition (ii) as follows:

$$S(s+t) = e^{\mu(s+t)} T(s+t) = e^{\mu s} e^{\mu t} T(s) T(t) = e^{\mu s} T(s) e^{\mu t} T(t) = S(s) S(t).$$

Finally, for all  $f \in X$ , we have

$$\begin{aligned} \|S(t)f - f\| &= \|e^{\mu t} T(t)f - f\| = \|e^{\mu t} T(t)f - e^{\mu t} f + e^{\mu t} f - f\| \\ &\leq \|e^{\mu t} T(t)f - e^{\mu t} f\| + \|e^{\mu t} f - f\| \\ &= e^{\mu t} \|T(t)f - f\| + |e^{\mu t} - 1| \|f\| \\ &\rightarrow 0 \text{ as } t \rightarrow 0^+. \end{aligned}$$

Hence condition (iii) is satisfied, completing the requirements of Definition 2.4.1 for a  $C_0$ -semigroup.

The bound given for  $\|S(t)\|$  is easily established, as shown below:

$$\|S(t)\| = \|e^{\mu t} T(t)\| = e^{\mu t} \|T(t)\| \leq e^{\mu t} M e^{\omega t} = M e^{(\omega + \mu)t} \text{ for } t \geq 0.$$

All that remains is to determine the generator of this semigroup, which we shall denote by  $B$ . Applying the method used in Definition 2.4.8, for any  $f \in D(A)$ , we have

$$\begin{aligned} \frac{S(t) - I}{t} f &= \frac{e^{\mu t} T(t) - I}{t} f = e^{\mu t} \frac{(T(t) - I)}{t} f + \frac{e^{\mu t} - 1}{t} f \\ &\rightarrow Af + \mu f = (A + \mu I) f \text{ as } t \rightarrow 0^+, \end{aligned}$$

where we have used L'Hôpital's rule to obtain the limit of the second term. Therefore  $D(A) \subseteq D(B)$  and  $Bf = (A + \mu I)f$  for  $f \in D(A)$ . Conversely, for  $f \notin D(A)$ , the limit of the right-hand side does not exist and hence neither does the limit of the left-hand side, implying that  $f \notin D(B)$ . Therefore the semigroup  $(S(t))_{t \geq 0}$ , must have generator  $B = A + \mu I$  with domain  $D(B) = D(A)$ .  $\square$

**Theorem 2.4.11.** *Let  $(T(t))_{t \geq 0}$  be a  $C_0$ -semigroup on a Banach space  $X$ , with generator  $A$ . Then, for all  $f \in D(A)$ , we have*

$$\begin{aligned} T(t)f \in D(A) \text{ and } A(T(t)f) &= T(t)(Af) \text{ for all } t \geq 0, \\ \frac{d}{dt} \{T(t)f\} &= A(T(t)f) = T(t)(Af), \end{aligned}$$

where the derivative is the strong derivative with respect to the norm on  $A$ , two-sided for  $t > 0$  and right-sided at  $t = 0$ .

*Proof.* See [14, Theorem 2.12].  $\square$

**Theorem 2.4.12.** *Let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$  on a Banach space  $X$ . Then  $A$  is a closed operator (Definition 2.3.1) with domain  $D(A)$ , which is dense in  $X$ .*

*Proof.* See [14, Theorem 2.13].  $\square$

**Lemma 2.4.13.** *Let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$  on a Banach space  $X$ . Then, for all  $t \geq 0$  and  $f \in X$ , we have*

$$\int_0^t T(s)f \, ds \in D(A),$$

with

$$T(t)f - f = A \int_0^t T(s)f \, ds.$$

Moreover, if  $f \in D(A)$ , we have

$$T(t)f - f = A \int_0^t T(s)f \, ds = \int_0^t T(s)Af \, ds.$$

*Proof.* See [28, Chapter 2, Lemma 1.3].  $\square$

**Theorem 2.4.14.** *Let  $(T(t))_{t \geq 0}$  and  $(S(t))_{t \geq 0}$  be two  $C_0$ -semigroups on the Banach space  $X$ . Supposing that these two semigroups share the generator  $A$ , then they are in fact the same semigroup, that is  $T(t)f = S(t)f$  for all  $t \geq 0$  and  $f \in X$ .*

*Proof.* See [68, Theorem 2.6].  $\square$

**Theorem 2.4.15.** *Let  $(T(t))_{t \geq 0}$  be a  $C_0$ -semigroup on a Banach space  $X$ . Suppose that the semigroup satisfies the bound (2.9) and has generator  $A$ . If  $\lambda > \omega$ , then  $\lambda \in \rho(A)$ , the resolvent operator is given by*

$$R(\lambda, A)f = \int_0^\infty e^{-\lambda s} T(s)f \, ds \text{ for all } f \in X,$$

and we have

$$\|R(\lambda, A)\| \leq \frac{M}{\lambda - \omega}.$$

*Proof.* See [28, Chapter 2, Theorem 1.10].  $\square$

**Definition 2.4.16.** Let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup. Then, for sufficiently large  $\lambda > 0$ , we define the *Yosida approximation*  $\mathcal{A}_\lambda$  of  $A$  by

$$\mathcal{A}_\lambda = \lambda^2 R(\lambda, A) - \lambda I = \lambda A R(\lambda, A).$$

- For large enough  $\lambda$ , we have  $\lambda \in \rho(A)$ . Therefore  $R(\lambda, A) \in B(X)$  and hence  $\mathcal{A}_\lambda \in B(X)$  for such values of  $\lambda$ ;
- The equality above is justified as follows:

$$\begin{aligned}\lambda^2 R(\lambda, A) - \lambda I &= \lambda(\lambda I - A)R(\lambda, A) + \lambda AR(\lambda, A) - \lambda I \\ &= \lambda I + \lambda AR(\lambda, A) - \lambda I \\ &= \lambda AR(\lambda, A);\end{aligned}$$

- The numerical analogue of the Yosida approximation is

$$\frac{\lambda^2}{\lambda - a} - \lambda = \frac{\lambda^2 - \lambda(\lambda - a)}{\lambda - a} = \frac{\lambda a}{\lambda - a} \rightarrow a \text{ as } \lambda \rightarrow \infty.$$

These points suggest that the Yosida approximations may provide bounded linear approximations to our generator  $A$  and that these approximations improve as  $\lambda$  increases. In the following lemma we shall consider this further.

**Lemma 2.4.17.** *Let  $A : D(A) \subseteq X \rightarrow X$  be a closed linear operator with  $D(A)$  dense in the Banach space  $X$ . Suppose that there exist  $\omega \in \mathbb{R}$  and  $M > 0$  such that  $[\omega, \infty) \subset \rho(A)$  and  $\|\lambda R(\lambda, A)\| \leq M$  for all  $\lambda \geq \omega$ . Then the following statements hold as  $\lambda \rightarrow \infty$ :*

- (i)  $\lambda R(\lambda, A)f \rightarrow f$  for all  $f \in X$ ;
- (ii)  $\lambda AR(\lambda, A)f = \lambda R(\lambda, A)Af \rightarrow Af$  for all  $f \in D(A)$ .

*Proof.* See [28, Chapter 2, Lemma 3.4]. □

We have now reached the point where we shall introduce the Hille–Yosida theorem. As mentioned previously, this theorem, and its generalisation are perhaps the most significant in the theory of semigroups. They give the user both necessary and sufficient conditions for the operator  $A$  to be the generator of a strongly continuous semigroup. Although we do not apply these results in the work that follows, we include them due to their significance to the field. We begin with the classical Hille–Yosida theorem, which applies in the case of a contraction semigroup.

**Theorem 2.4.18.** (Contraction Semigroup; Hille [36], Yosida [82]) *The operator  $A$  generates a  $C_0$ -semigroup of contractions  $(T(t))_{t \geq 0}$ , that is  $A \in \mathcal{G}(1, 0; X)$ , if and only if*

- (i)  $A$  is a closed linear operator with domain  $D(A)$ , which is dense in  $X$ ;
- (ii) for all real numbers  $\lambda > 0$ , we have  $\lambda \in \rho(A)$  and

$$\|R(\lambda, A)\| \leq \frac{1}{\lambda}.$$

*Proof.* See [28, Chapter 2, Theorem 3.5].  $\square$

The following theorem extends that of Hille and Yosida to cover general semigroups. Even though it is a result due to others, it often named as the Hille–Yosida theorem in the literature.

**Theorem 2.4.19.** (General Semigroup; Feller [30], Miyadera [61], Philips [72])  
*Let  $X$  be a Banach space. Then  $A \in \mathcal{G}(M, \omega; X)$  if and only if*

- (i)  *$A$  is a closed linear operator with domain  $D(A)$ , which is dense in  $X$ ;*
- (ii) *for all real numbers  $\lambda > \omega$ , we have  $\lambda \in \rho(A)$  and for  $n = 1, 2, \dots$*

$$\|(R(\lambda, A))^n\| \leq \frac{M}{(\lambda - \omega)^n}.$$

*Proof.* The proof of the general case is an adaption of that used in the previous theorem for contraction semigroups. This involves the application a rescaling technique, similar to that of Theorem 2.4.3, and the introduction of a new norm, under which our general semigroup becomes a contraction semigroup. We are then able to apply Theorem 2.4.18. For details, see [28, Chapter 2, Theorem 3.8].  $\square$

In the general case, establishing whether or not a given operator  $A$  satisfies the conditions of Theorem 2.4.19 is usually a complicated task. In particular, computing the powers of the resolvent and establishing condition (ii) often proves intractable. However, in the case of a contraction semigroup the task is more likely to be achievable. Such semigroups are significant as they arise regularly in practice. This is particularly true where our system has some physical quantity which is non-increasing, and the norm is chosen to provide a measure of this quantity. We therefore spend some time considering contraction semigroups and their generators further. As mentioned, the difficulty in applying the Hille–Yosida theorem in practice is often due to the requirement to calculate the resolvent operator. It is possible to characterise the generators of contraction semigroups without recourse to the resolvent operator. However, before we do so, it is necessary to define some further terminology.

**Definition 2.4.20.** Let  $X$  be a Banach space and  $A : D(A) \subseteq X \rightarrow X$  a linear operator.

- $A$  is *dissipative* if

$$\|(\lambda I - A)f\| \geq \lambda \|f\| \quad \text{for all } \lambda > 0 \text{ and } f \in D(A);$$

- $A$  is  *$m$ -dissipative* if it is dissipative and

$$\text{Range}(\lambda I - A) = X \quad \text{for all } \lambda > 0.$$

**Theorem 2.4.21.** (The Lumer-Phillips Characterisation of Generators of Contraction Semigroups) *The linear operator  $A$  generates a  $C_0$ -semigroup of contractions ( $A \in \mathcal{G}(1, 0; X)$ ) if and only if*

- (i)  $A$  is a closed operator with domain  $D(A)$ , which is dense in  $X$ ;
- (ii)  $A$  is  $m$ -dissipative.

*Proof.* See [68, Chapter 1, Theorem 4.3]. □

### 2.4.4 Constructing the Semigroup

Supposing we have an operator  $A$ , which we have identified as the generator of a  $C_0$ -semigroup, then the question which naturally arises is how we obtain the semigroup itself. In the case that our generator is a bounded operator  $A \in B(X)$ , then the associated semigroup  $(T(t))_{t \geq 0}$  is simply given by

$$T(t) = \exp(tA) = \sum_{n=0}^{\infty} \frac{t^n A^n}{n!}. \quad (2.12)$$

However, when the generator  $A$  is unbounded, as is often the case in practical applications, we cannot be certain of the convergence of this series. Therefore, if semigroup theory is to be usefully applied in such cases, then alternative construction methods must be sought. The first approach we shall outline comes from the work of Hille, and takes as its inspiration the common limit definition of the standard scalar exponential function. For a real or complex scalar  $a$ , it is well known that

$$\exp(ta) = (\exp(-ta))^{-1} = \left\{ \lim_{n \rightarrow \infty} \left( 1 - \frac{t}{n} a \right)^n \right\}^{-1} = \lim_{n \rightarrow \infty} \left\{ \left( 1 - \frac{t}{n} a \right)^{-1} \right\}^n.$$

Similarly to the bounded case, where the series definition of the exponential function gave us our semigroup, we might hope to obtain the semigroup by replacing the scalar  $a$  with the operator  $A$  in the above relation as follows:

$$\exp(tA)f = \lim_{n \rightarrow \infty} \left\{ \left[ \left( I - \frac{t}{n} A \right)^{-1} \right]^n \right\} f = \lim_{n \rightarrow \infty} \left\{ \left[ \frac{n}{t} \left( \frac{n}{t} I - A \right)^{-1} \right]^n \right\} f,$$

for  $f \in X$ . It is worth noting the appearance of a resolvent operator on the right-hand side of the above equation. This idea is formalised in the following theorem.

**Theorem 2.4.22.** *Let  $X$  be a Banach space and let  $A \in \mathcal{G}(M, \omega; X)$  generate the  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ . Then, for all  $f \in X$*

$$T(t)f = \lim_{n \rightarrow \infty} \left\{ \left[ \frac{n}{t} R \left( \frac{n}{t}, A \right) \right]^n \right\} f,$$

where convergence is uniform with respect to  $t$  on  $[0, t_0]$ , for any  $t_0 > 0$ .

*Proof.* See [68, Chapter 1, Theorem 8.3].  $\square$

This representation of the semigroup provides us with the following useful result for characterising positive semigroups.

**Theorem 2.4.23.** *Let  $X$  be a Banach space with positive cone  $X_+$ . Then the  $C_0$ -semigroup  $(T(t))_{t \geq 0}$  generated on  $X$  by  $A \in \mathcal{G}(M, \omega; X)$  is positive, if and only if, the resolvent,  $R(\lambda, A)$ , of the generator is positive for all sufficiently large  $\lambda$ .*

*Proof.* See [28, Chapter 6, Theorem 1.8].  $\square$

The second approach we shall consider was provided by Yosida. The method relies on approximating the generator  $A$  by the family of Yosida approximations  $\{\mathcal{A}_\lambda\}$  as defined in Definition 2.4.16. For sufficiently large values of  $\lambda$  the operators  $\mathcal{A}_\lambda$  are bounded and therefore generate a  $C_0$ -semigroup via (2.12). It is our hope that by taking these semigroups and letting  $\lambda \rightarrow \infty$ , we shall obtain our desired semigroup. The success of this approach is confirmed in the following theorem.

**Theorem 2.4.24.** *Let  $X$  be a Banach space and let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ . Then, for all  $f \in D(A)$*

$$\lim_{\lambda \rightarrow \infty} \mathcal{A}_\lambda f = Af,$$

and

$$T(t)f = \lim_{\lambda \rightarrow \infty} \exp(t\mathcal{A}_\lambda) f \text{ for all } t \geq 0 \text{ and } f \in X.$$

*Proof.* The proof for the case when  $A \in \mathcal{G}(1, 0; X)$  is covered in the standard proof of the Hille–Yosida theorem; see [68, Chapter 1, Lemma 3.3]. The general case when  $A \in \mathcal{G}(M, \omega; X)$  is handled by a renorming and rescaling; for details see [68, Chapter 1, Theorem 5.5].  $\square$

## 2.5 Evolution Equations in a Banach Space

In order to bring the theory of semigroups to bear on our problems of interest, we must frame them in the correct setting. As such we will be interested in abstract differential equations involving Banach-space-valued functions  $f : [0, T) \rightarrow X$  of the form

$$\frac{d}{dt} f = F, \quad f(0) = f_0, \quad (2.13)$$

where  $F : (0, T) \rightarrow X$  (for some  $0 < T \leq \infty$ ) and  $f_0 \in X$ . As a first step we must define exactly what is meant when we talk about a solution of (2.13). We now introduce the notions of *strong*, *mild* and *weak* solutions of (2.13), and explain how they relate to one another.

**Definition 2.5.1.** A *strong* solution of (2.13) is a continuous function  $f : [0, T] \rightarrow X$  that is continuously differentiable on  $(0, T)$  and satisfies (2.13) directly.

Assuming that  $F$  is integrable, then integrating equation (2.13) between 0 and  $0 < t < T$  we obtain

$$f(t) = f_0 + \int_0^t F(s) \, ds. \quad (2.14)$$

**Definition 2.5.2.** A function  $f : [0, T] \rightarrow X$  is a *mild* solution of (2.13) if it is strongly continuous and satisfies (2.14) for all  $t \in (0, T)$ .

*Remark 2.5.3.* We note that due to the fundamental theorem of calculus, any strong solution automatically satisfies the conditions for a mild solution, however the converse is not true as  $f$  may not be differentiable.

We have one further form of solution to introduce, which is referred to as a *weak* solution. Such solutions will occur in the subsequent chapters as the limits of our numerical scheme.

**Definition 2.5.4.** A function  $f : [0, T] \rightarrow X$  is a *weak* solution of (2.13), if for all  $\phi \in X'$  (where  $X'$  denotes the dual space of  $X$ ) we have that  $t \rightarrow \langle f(t), \phi \rangle$  is locally integrable in  $(0, T)$  and

$$\int_0^T \langle f(s), \phi \rangle \frac{d}{ds} \psi(s) \, ds = -\langle f_0, \phi \rangle \psi(0) - \int_0^T \langle F(s), \phi \rangle \psi(s) \, ds, \quad (2.15)$$

for all  $\psi \in C^\infty([0, T])$  with compact support, where  $\langle g, \phi \rangle$  denotes the duality pairing of  $g \in X$  and  $\phi \in X'$ .

*Remark 2.5.5.* If  $D \subseteq X'$  is dense in the weak-\* topology, then it is sufficient to show that (2.15) holds for all  $\phi \in D$  to establish  $f : [0, T] \rightarrow X$  as a *weak* solution of (2.13); see [19, Definition 1.9].

We have already noted that strong solutions automatically provide us with mild solutions. The following result gives us the equivalence of mild and weak solutions, when our  $F$  is of a suitable form.

**Theorem 2.5.6.** *Let  $F : (0, T) \rightarrow X$  be integrable. Then given a solution  $f : [0, T] \rightarrow X$  of (2.13), in the sense of either Definition 2.5.2 or Definition 2.5.4, we may alter that solution on a set of measure zero and obtain a solution of the other type.*

*Proof.* See [19, Theorem 1.20] □

### 2.5.1 Abstract Cauchy Problem

Having introduced the idea of an abstract differential equation in a Banach space, we now consider a specific type of equation where the function  $F$  takes a particular form.

**Definition 2.5.7.** Let  $X$  be a Banach space and let  $A : D(A) \subseteq X \rightarrow X$  be some linear operator. Then the *homogeneous abstract Cauchy problem* (ACP) associated with this operator is

$$\frac{d}{dt}u(t) = Au(t) \quad (t > 0); \quad u(0) = u_0, \quad (2.16)$$

where  $u_0$  is some given fixed element of  $X$ .

**Theorem 2.5.8.** Let  $X$  be a Banach space and let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ . Then if  $u_0 \in D(A)$ , the homogeneous ACP (2.16) associated with  $A$  has the unique strong solution

$$u(t) = T(t)u_0 \quad (t \geq 0).$$

Note that we require a strong solution to the ACP to satisfy  $u(t) \in D(A)$  for all  $t \geq 0$ .

*Proof.* See [14, Theorem 2.40 and Theorem 2.41]. □

The strong solution obtained above requires that the initial value  $u_0$  be in  $D(A)$ . Indeed, from the definition of  $D(A)$  we have a strong solution if and only if  $u_0 \in D(A)$ . For  $u_0 \in X \setminus D(A)$  the function  $u(t) = T(t)u_0$  is continuous but, in general, not differentiable. However the semigroup can still provide us with a solution in such cases.

**Definition 2.5.9.** A continuous function  $u : \mathbb{R}_+ \rightarrow X$  is a *mild solution* of the ACP (2.16) if  $\int_0^t u(s) ds \in D(A)$  for all  $t \geq 0$  and

$$u(t) = u_0 + A \int_0^t u(s) ds, \quad (2.17)$$

where  $u_0$  is some given fixed element of  $X$ .

**Theorem 2.5.10.** Let  $X$  be a Banach space and let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ . Then, for every  $u_0 \in X$ ,  $u(t) = T(t)u_0$  provides the unique mild solution (as in Definition 2.5.9) to the homogeneous ACP (2.16).

*Proof.* See [28, Chapter 2, Proposition 6.4]. □

*Remark 2.5.11.* If we compare the definition of a mild solution for the abstract Cauchy problem in Definition 2.5.9 with that provided earlier in Definition 2.5.2, then we may see that it differs from what we might expect. In particular, the operator  $A$  could be expected to appear within the integral in Definition 2.5.9. However, for general  $u_0 \in X$  we cannot guarantee that  $u(t) \in D(A)$  for all  $t \geq 0$ . Hence we may not be able to apply  $A$  as desired. In the case that  $u_0 \in D(A)$ , as will be the case when we utilise Theorem 2.4.15, then by Lemma 2.4.13 we may pass  $A$  through the integral in (2.17) to obtain the form expected from Definition 2.5.2 and indeed in such cases the unique strong and mild solutions coincide.

Often our equations of interest are not easily expressed in a form like equation (2.16), usually this will involve additional terms on the right-hand side. We now consider a number of alternative forms of equation which will occur in our analysis and provide an overview of the associated theory we shall require.

**Definition 2.5.12.** Let  $X$  be a Banach space,  $A: D(A) \subseteq X \rightarrow X$  a linear operator and  $\varphi: [0, T) \rightarrow X$  for some  $(0 < T \leq \infty)$ . Then an equation of the form

$$\frac{d}{dt}u(t) = Au(t) + \varphi(t) \quad (0 < t \leq T); \quad u(0) = u_0, \quad (2.18)$$

is known as an *inhomogeneous abstract Cauchy problem* (iACP).

**Definition 2.5.13.** When we refer to a *strong* solution of (2.18) we mean a function  $u: [0, T) \rightarrow X$  with the usual properties of being (strongly) continuous on  $[0, T)$ , (strongly) differentiable on  $(0, T)$ , which satisfies (2.18) directly.

Let  $A$  generate the  $C_0$ -semigroup  $(T(t))_{t \geq 0}$  and suppose that  $u$  is a (strong) solution to equation (2.18). We may define the function  $h(s) = T(t-s)u(s)$ , which is differentiable on  $0 < s < t$  and we then have

$$\begin{aligned} \frac{d}{ds}h(s) &= -AT(t-s)u(s) + T(t-s)u'(s) \\ &= -AT(t-s)u(s) + T(t-s)Au(s) + T(t-s)\varphi(s) \\ &= -AT(t-s)u(s) + AT(t-s)u(s) + T(t-s)\varphi(s) \\ &= T(t-s)\varphi(s). \end{aligned} \quad (2.19)$$

Assuming that  $\varphi \in L_1((0, T), X)$  then  $T(t-s)\varphi(s)$  is integrable. If we then integrate equation (2.19) between 0 and  $t$  we obtain

$$u(t) = T(t)u_0 + \int_0^t T(t-s)\varphi(s) ds. \quad (2.20)$$

For each  $\varphi \in L_1((0, T), X)$ , the function  $u(t)$  defined by equation (2.20) is continuous on  $[0, T]$ , but not necessarily differentiable. This raises the prospect of a weaker form of solution than presented in Definition 2.5.13.

**Definition 2.5.14.** By a *mild* solution to (2.18), we mean a (strongly) continuous function  $u : [0, T) \rightarrow X$  such that  $\int_0^t u(s) ds \in D(A)$  for  $t \in [0, T)$  and

$$u(t) = u_0 + A \int_0^t u(s) ds + \int_0^t \varphi(s) ds, \quad \text{for } (0 \leq t < T). \quad (2.21)$$

*Remark 2.5.15.* Comparing Definition 2.5.14 to Definition 2.5.2 we again see a difference as in the homogeneous case, where we may expect the operator  $A$  to appear inside the integral. However, this may be problematic in general as we have no reason to expect  $u(t) \in D(A)$  for all admissible  $t$ . That being said, in the cases in which we will apply the notion of a mild solution as in Definition 2.5.14, the operator  $A$  will be bounded on all of  $X$  and so such an operation can be justified by Lemma 2.3.4. It is easily verified that any strong solution of equation (2.18) automatically satisfies Definition 2.5.14 and so provides a mild solution.

**Theorem 2.5.16.** *Let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ . Then for any  $\varphi \in L_1((0, T), X)$  and  $u_0 \in D(A)$ , the inhomogeneous ACP (2.18) has a unique mild solution, which is given by (2.20).*

*Proof.* See [68, Chapter 4, Corollary 2.2, Definition 2.3] and [10, Proposition 3.31].  $\square$

We may now ask what additional conditions can be imposed in order for our mild solution to satisfy the stricter definition of a strong solution. The following theorem provides us with sufficient conditions such that our solution  $u(t)$  satisfies Definition 2.5.13.

**Theorem 2.5.17.** *Let  $A : D(A) \subseteq X \rightarrow X$  be the generator of a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ . If  $\varphi$  is differentiable almost everywhere on  $[0, T]$  and  $\varphi' \in L_1((0, T), X)$ , then for each  $u_0 \in D(A)$ , the inhomogeneous ACP (2.18) has a unique strong solution on  $[0, T]$  (satisfying Definition 2.5.1), which is given by (2.20).*

*Proof.* See [68, Chapter 4, Corollary 2.2 and Corollary 2.10].  $\square$

*Remark 2.5.18.* Any  $\varphi$  satisfying the conditions of Theorem 2.5.17 must also satisfy those set out in Theorem 2.5.16. Therefore, in cases as described in Theorem 2.5.17 there must also be a unique mild solution, which coincides with the strong solution.

## 2.5.2 Perturbations

When formulating our equation of interest as an abstract Cauchy problem, it is common that the terms which should appear on the right-hand side of equation (2.16) are more naturally expressed as two or more separate operators, perhaps

due to the differing nature of the effects they are representing. This results in an equation of the form

$$\frac{d}{dt}u(t) = Au(t) + Bu(t) \quad (t > 0); \quad u(0) = u_0.$$

Very often checking the conditions of Theorem 2.4.19 directly for  $A + B$  would prove intractable. In situations such as this, it is often easier to consider the operators  $A$  and  $B$  individually, making use of a set of theorems known as *perturbation results*. In most of these results it is assumed that one of the individual operators, say  $A$ , generates a  $C_0$ -semigroup. The question then arises under what conditions on  $B$  the combined operator  $A + B$  (or some related operator) forms a generator of a  $C_0$ -semigroup.

Perhaps the most obvious example in which we might expect a positive answer, is the case where the operator  $B$  is bounded, and such a case is covered in the following theorem.

**Theorem 2.5.19.** *Let the linear operator  $(A, D(A))$  generate a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$ , satisfying the bound (2.9) on a Banach space  $X$ . If  $B \in B(X)$ , i.e.  $B$  is a bounded linear operator from  $X$  into  $X$  then the sum  $A + B$  with  $D(A + B) = D(A)$  generates a  $C_0$ -semigroup,  $(S(t))_{t \geq 0}$ , satisfying*

$$\|S(t)\| \leq Me^{(\omega + M\|B\|)t} \quad \text{for } t \geq 0.$$

*Proof.* See [28, Chapter 3, Theorem 1.3]. □

**Theorem 2.5.20.** *Let  $(A, D(A))$  and  $(A + B, D(A))$  respectively generate the  $C_0$ -semigroups  $(T(t))_{t \geq 0}$  and  $(S(t))_{t \geq 0}$  on the Banach space  $X$ , where  $B \in B(X)$ . Then for all  $f \in X$  and  $t \geq 0$ , the semigroups satisfy Duhamel's equation, that is*

$$S(t)f = T(t)f + \int_0^t T(t-s)BS(s)f \, ds.$$

*Proof.* See [28, Chapter 3, Corollary 1.7]. □

**Theorem 2.5.21.** *Suppose that the  $C_0$ -semigroup  $(S(t))_{t \geq 0}$  is generated by the operator  $(A + B, D(A))$ , where  $(A, D(A))$  generates the  $C_0$ -semigroup  $(T(t))_{t \geq 0}$  and  $B \in B(X)$ . Then the semigroup  $(S(t))_{t \geq 0}$  can be obtained as follows:*

$$S(t) = \sum_{n=0}^{\infty} S_n(t), \tag{2.22}$$

where  $S_0(t) := T(t)$  and

$$S_{n+1}(t)f := \int_0^t T(t-s)BS_n(s)f \, ds, \quad t \geq 0, f \in X.$$

The series (2.22), known as the *Dyson–Phillips series* [27], converges in the operator norm on  $B(X)$  and uniformly for  $t$  on compact intervals of  $[0, \infty)$ .

*Proof.* See [28, Chapter 3, Theorem 1.10].  $\square$

For some of the applications in the later chapters, the requirement that  $B$  be bounded will turn out to be too restrictive. We therefore turn to an alternative perturbation result, namely the Kato–Voigt perturbation theorem. This result does not rely on  $B$  being bounded. However, in removing this restriction we lose  $A + B$  as our generator and instead we can only say that some extension of  $A + B$  is a generator.

**Theorem 2.5.22.** (Kato–Voigt Perturbation Theorem) *Let  $X = L_1(\Omega, \mu)$  and suppose the linear operators  $A$  and  $B$  satisfy the conditions*

- (i)  $(A, D(A))$  generates a substochastic semigroup  $(G_A(t))_{t \geq 0}$  on  $X$ ;
- (ii)  $B$  is a positive linear operator with  $D(A) \subseteq D(B)$ ;
- (iii) For all  $f \in D(A)_+$ ,

$$\int_{\Omega} (Af + Bf) d\mu \leq 0.$$

*Then, there exists an extension  $(K, D(K))$  of the operator  $(A + B, D(A))$ , which generates a substochastic semigroup  $(G_K(t))_{t \geq 0}$ .*

*Proof.* See [10, Corollary 5.17].  $\square$

*Remark 2.5.23.* For reasons which will become apparent in the upcoming definition, it is common to express condition (iii) in the form

$$\int_{\Omega} (A + B)f d\mu = -c(f) \text{ for } f \in D(A)_+, \quad (2.23)$$

where  $c$  is some non-negative linear functional defined on  $D(A)$ .

A practical downside of this result is that it guarantees only the existence of a generator  $K$ , and provides no indication of how this operator relates to  $A + B$ . The nature of the generator  $K$  is closely related to the concept of semigroup honesty, which we now define.

**Definition 2.5.24.** The positive semigroup  $(G_K(t))_{t \geq 0}$ , generated by the extension  $K$  of  $A + B$  from Theorem 2.5.22, is *honest* if the linear functional  $c$ , given by (2.23), extends to  $D(K)$ , and for all  $u_0 \in D(K)_+$ , the non-negative solution  $u(t) = G_K(t)u_0$  to

$$\frac{d}{dt}u(t) = Ku(t), \quad t > 0; \quad u(0) = u_0,$$

satisfies

$$\frac{d}{dt} \|u(t)\| = \frac{d}{dt} \int_{\Omega} u(t) \, d\mu = -c(u(t)),$$

where  $\|\cdot\|$  is the norm on the space  $X$  from Theorem 2.5.22.

**Lemma 2.5.25.** *The functional  $c$ , given by (2.23), extends to a non-negative continuous linear functional on  $D(K)$*

*Proof.* See [10, Theorem 6.8]. □

**Theorem 2.5.26.** *The semigroup  $(G_K(t))_{t \geq 0}$  is honest if and only if  $K = \overline{A + B}$ .*

*Proof.* See [10, Theorem 6.13]. □

*Remark 2.5.27.* Some results exist which allow us to obtain the generator  $K$  and in Chapter 3 we shall apply these results. However, their explanation is heavily dependent on the specific application and involves material which is not suitably covered here. Therefore, we leave the introduction of the aforementioned results until the relevant part of Chapter 3, where they appear as Theorem 3.2.4 and Lemma 3.2.6.

**Theorem 2.5.28.** *Let  $D$  be a core (Definition (2.3.13)) for the operator  $A$ . If  $(G(t))_{t \geq 0}$  is another positive semigroup, generated by an extension of  $(A + B, D)$ , then  $G(t) \geq G_K(t)$ , where  $(G(t))_{t \geq 0}$  is the semigroup generated by  $K = \overline{A + B}$ .*

*Proof.* See [10, Proposition 5.7]. □

### 2.5.3 Systems of Equations

The particular problems we shall be considering involve multiple governing equations, describing quantities which are fundamentally different in nature. When looking to reformulate these equations as abstract differential equations, of the type we have been describing, then we find that the differing nature of the equations means that different spaces are best suited for their analysis. However, just as it is possible to express a system of  $n$  scalar differential equations as a single equation in  $\mathbb{R}^n$  using matrix notation, we may transform our system of abstract equations into a single equation of the form (2.16). The space  $X$  is now a product space, Definition 2.1.8, and the operator  $A$  takes the form of a matrix whose entries are themselves operators which map from and to the relevant spaces.

In our case, as we shall be considering a coupled set of 2 equations, we end up with a  $2 \times 2$  operator matrix. The specific nature of the problem means that the matrix in question will be of upper triangular form. The following result gives sufficient conditions for such an operator to be a generator, as well as providing the semigroup generated.

**Theorem 2.5.29.** *Let  $X$  and  $Y$  be Banach spaces. Consider the operator matrix*

$$\mathbf{A} = \begin{pmatrix} A & B \\ 0 & D \end{pmatrix}.$$

*Suppose that the following hold for the linear operators  $A$ ,  $B$  and  $D$ :*

- (i)  $A : D(A) \subseteq X \rightarrow X$  generates a  $C_0$ -semigroup  $(T(t))_{t \geq 0}$  on  $X$ ;
- (ii)  $D : D(D) \subseteq Y \rightarrow Y$  generates a  $C_0$ -semigroup  $(S(t))_{t \geq 0}$  on  $Y$ ;
- (iii)  $B : D(B) \subseteq Y \rightarrow X$  is relatively  $D$ -bounded;
- (iv)  $(\mathbf{A}, D(\mathbf{A}))$  is a closed operator;
- (v) the operator  $\tilde{R}(t) : D(D) \subseteq Y \rightarrow X$  given by  $\tilde{R}(t)f = \int_0^t T(t-s)BS(s)f \, ds$ , has a unique extension  $R(t) \in B(Y, X)$  which is uniformly bounded as  $t \searrow 0$ .

*Then  $\mathbf{A}$ , with domain  $D(\mathbf{A}) = D(A) \times D(D) \subseteq X \times Y$ , generates a strongly continuous semigroup  $(\mathbf{T}(t))_{t \geq 0}$  on the product space  $X \times Y$ . Moreover, this semigroup is given by*

$$\mathbf{T}(t) := \begin{pmatrix} T(t) & R(t) \\ 0 & S(t) \end{pmatrix}, \quad t \geq 0.$$

*Proof.* See [63, Proposition 3.1]. □

In this chapter we have introduced many of the relevant concepts and the theory which we shall require for our analysis in the rest of the thesis. In the next chapter we will introduce our new model and carry out the rigorous analysis of it, using the methods outlined here.

# Chapter 3

## A Mixed Discrete–Continuous Fragmentation Model: Introduction and Analysis

### 3.1 Introduction

Many mathematical models of fragmentation consider the mass of the particles as a continuous variable. However, as discussed in Chapter 1, we can encounter difficulties with such models when the fragmentation rate is unbounded at zero. The unbounded fragmentation rate results in a runaway fragmentation process and an unaccounted mass loss due to the phenomenon known as ‘shattering’ [57]. Although at the mesoscopic scale the continuum model may provide an adequate representation of matter, on closer inspection we might expect there to be some minimum fundamental unit (monomer) from which all larger particles are built up. Such a structure would be inconsistent with the runaway fragmentation encountered in the shattering phenomenon.

In this chapter we shall present a mixed discrete/continuous fragmentation model as a solution to the problem of shattering. The smaller particles are considered to be comprised of collections of monomers. Through suitable scaling, the monomers can be assumed to have unit mass and therefore the smaller particles take positive integer mass, up to a cut-off value  $N \in \mathbb{N}$ . However, above this cut-off particle mass is considered as a continuous variable. A set-up such as this produces a dual regime model, with a discrete mass regime below the cut-off and a continuous mass regime above.

Let us denote by  $u_C(x, t)$  the particle mass density within the continuous mass regime. The evolution of  $u_C(x, t)$  is then governed by the continuous multiple fragmentation equation below:

$$\begin{aligned} \frac{\partial u_C(x, t)}{\partial t} &= -a(x)u_C(x, t) + \int_x^\infty a(y)b(x|y)u_C(y, t) dy, \quad x > N, t > 0, \\ u_C(x, 0) &= c_0(x). \end{aligned} \quad (3.1)$$

As with equation (1.5), the function  $a(x)$  provides the fragmentation rate for a particle of mass  $x$ , whilst  $b(x|y)$  represents the distribution of particles of mass  $x > N$  resulting from the break-up of a particle of mass  $y > x$ . The functions  $a$  and  $b$  are assumed to be non-negative measurable functions, defined on  $(N, \infty)$  and  $(N, \infty) \times (N, \infty)$ , respectively. We also require  $b(x|y) = 0$  for  $x > y$ , since no particle resulting from a fragmentation event can have a mass exceeding the original parent particle. Finally,  $c_0(x)$  details the initial mass distribution within the continuous regime.

The explanation of each of the terms in equation (3.1) matches the one for the corresponding term from equation (1.5). The first term on the right-hand side of equation (3.1) is a loss term; accounting for those particles of mass  $x > N$  which are lost due to their fragmentation into smaller particles. The second term, involving the integral, is a gain term and corresponds to the increase we see in particles of mass  $x$ , due to the break-up of larger particles.

Turning our attention to the discrete mass regime, let  $u_{D_i}(t)$  denote the concentration of  $i$ -mer particles and  $u_D(t)$  the  $N$ -vector taking these values as entries. The change in the values  $u_{D_i}(t)$ ,  $i = 1, \dots, N$ , is governed by the equations:

$$\begin{aligned} \frac{du_{D_i}(t)}{dt} &= -a_i u_{D_i}(t) + \sum_{j=i+1}^N a_j b_{i,j} u_{D_j}(t) + \int_N^\infty a(y) b_i(y) u_C(y, t) dy, \quad t > 0, \\ u_D(0) &= d_0. \end{aligned} \quad (3.2)$$

In the case of  $i = N$ , the second term becomes an empty sum and is taken to be 0. The values  $a_i$  give the rates at which  $i$ -mer particles fragment, with  $a_1 = 0$ . The quantities  $b_{i,j}$  give the expected number of  $i$ -mers produced from the fragmentation of a  $j$ -mer and the functions  $b_i(y)$  give the expected number of  $i$ -mers produced from the fragmentation of a particle of mass  $y > N$ . The underlying physics demands that each  $a_i$ ,  $b_{i,j}$  and  $b_i(y)$  be non-negative. Finally,  $d_0$  is the  $N$ -vector giving the initial mass distribution within the discrete regime.

Analogously to equation (3.1), the first term on the right-hand side of equation (3.2) is a loss term, accounting for the loss in  $i$ -mer particles due to their fragmentation into smaller particles. The remaining two terms are gain terms, with the term involving the summation giving the increase in  $i$ -mers due to the break-up of larger  $j$ -mers and the integral term representing production of new  $i$ -mers from the fragmentation of larger continuous mass particles.

In any fragmentation event, mass is simply redistributed from the larger particle to the smaller resulting particles, but the total mass involved should be conserved. This gives us the following two mass conservation conditions to supplement equations (3.1) and (3.2):

$$\int_N^y xb(x|y) dx + \sum_{j=1}^N jb_j(y) = y \text{ for } y > N, \quad (3.3)$$

$$\sum_{j=1}^{i-1} jb_{j,i} = i \text{ for } i = 2, \dots, N. \quad (3.4)$$

The condition (3.3) is an expression of mass conservation upon the fragmentation of a particle from the continuous mass regime. The integral term gives the expected mass accounted for by resulting particles remaining within the continuous mass regime, that is those with mass lying in the range  $N < x < y$ , whereas the summation term represents the expected total mass attributable to the resulting particles in the discrete mass regime, i.e. those taking an integer value from 1 to  $N$ . The equation (3.4) comes from the conservation of mass when a particle from the discrete mass regime breaks up. Only one term is required for this condition as when a particle of discrete mass fragments, all resulting particles must themselves lie within the discrete mass regime.

The necessity of these conditions can be seen from equations (3.1) and (3.2). If we integrate the right-hand side of (3.1) over  $(N, \infty)$  with respect to the measure  $x dx$  and if we multiply the right-hand side of (3.2) by  $i$  and then sum over  $i$  from 1 to  $N$ , then formally, the sum of these two quantities gives us the rate of change of the total mass. Equating the continuous and discrete components of the resulting expression to zero, provides us with the conditions (3.3) and (3.4) respectively. However, these conditions alone are insufficient to guarantee mass conservation since the validity of the associated calculation requires a degree of regularity from the solutions, which is not known a priori. Indeed, we can see this in Section 7.1 where a purely continuous model of the form (1.5), satisfying (1.6) (the continuous analogue of (3.3) and (3.4)) is shown to display a loss of mass. Calculations similar to those described above can be found in Lemma 3.5.2, where (3.3) can be seen in (3.28) and (3.4) in the first term of (3.26). It should be noted, that as opposed to the formal calculations described here, by the point we reach Lemma 3.5.2, we

have established the existence of solutions with sufficient regularity to justify the calculations appearing there.

## 3.2 Continuous Fragmentation Regime

Looking initially at equation (3.1), we shall conduct our analysis of this equation within the setting of the weighted Lebesgue space  $X_C = L_1((N, \infty), x dx)$ . This is an obvious choice of space in which to study the problem, as the norm  $\|\cdot\|_{X_C}$ , when applied to the particle mass density  $u_C$ , provides a measure of mass. From the terms of equation (3.1), we introduce the following expressions

$$(\mathcal{A}f)(x) = -a(x)f(x) \quad \text{and} \quad (\mathcal{B}f)(x) = \int_x^\infty a(y)b(x|y)f(y) dy \quad \text{for } x > N. \quad (3.5)$$

From these expressions we form the operators  $A_C$  and  $B_C$  as follows:

$$\begin{aligned} (A_C f)(x) &= (\mathcal{A}f)(x), & D(A_C) &= \{f \in X_C : A_C f \in X_C\}, \\ (B_C f)(x) &= (\mathcal{B}f)(x), & D(B_C) &= \{f \in X_C : B_C f \in X_C\}. \end{aligned}$$

The following result relates the given domains of these operators, allowing us to consider taking their sum  $A_C + B_C$ .

**Lemma 3.2.1.**  $D(A_C) \subseteq D(B_C)$  as  $\|B_C u\|_{X_C} \leq \|A_C u\|_{X_C}$  for  $u \in D(A_C)$ . Hence  $(A_C + B_C, D(A_C))$  is a well-defined operator.

*Proof.* Let  $f \in D(A_C)$ . Then

$$\begin{aligned} \|B_C f\|_{X_C} &= \int_N^\infty \left| \int_x^\infty a(y)b(x|y)f(y) dy \right| x dx \\ &\leq \int_N^\infty \left( \int_x^\infty a(y)b(x|y) |f(y)| dy \right) x dx \\ &= \int_N^\infty a(y) |f(y)| \left( \int_N^y x b(x|y) dx \right) dy \\ &\leq \int_N^\infty a(y) |f(y)| y dy = \|A_C f\|_{X_C}. \end{aligned} \quad (3.6)$$

Hence we have  $f \in D(B_C)$ , and so  $D(A_C) \subseteq D(B_C)$ . The final inequality follows since  $\int_N^y x b(x|y) dx \leq y$ , due to the mass conservation condition (3.3). This reflects the fact that upon fragmentation of a particle of mass  $y > N$ , the total mass of the resulting particles remaining within the continuous regime cannot exceed  $y$ .  $\square$

This allows us to form the operator  $A_C + B_C$  with domain  $D(A_C)$ . Equation (3.1) is then reformulated in the setting of  $X_C$  as the abstract Cauchy problem:

$$\frac{d}{dt}u_C(t) = K[u_C(t)], \quad t > 0; \quad u_C(0) = c_0 \in D(K), \quad (3.7)$$

where  $K$  is some extension of the operator  $A_C + B_C$ . The Kato–Voigt perturbation theorem (Theorem 2.5.22) will allow us to prove the existence of such an operator  $K$ , which generates a semigroup.

**Theorem 3.2.2.** *There exists an extension  $(K, D(K))$  of  $(A_C + B_C, D(A_C))$ , which generates a substochastic semigroup  $(G_K(t))_{t \geq 0}$ .*

*Proof.* To establish this result we show that the three conditions set out in Theorem 2.5.22 are satisfied for our particular operators  $A_C$  and  $B_C$ .

1. It is clear that  $(A_C, D(A_C))$  generates a substochastic semigroup  $(G_{A_C}(t))_{t \geq 0}$ , where  $(G_{A_C}(t)f)(x) = \exp(-a(x)t)f(x)$ .
2. We have shown in Lemma 3.2.1 that  $D(A_C) \subseteq D(B_C)$ . The non-negativity of  $a$  and  $b$  imply that  $B_C$  a positive operator, so that  $B_C f \in X_{C+}$  for all  $f \in D(B_C)_+$ .
3. For all  $f \in D(A_C)_+$  we have that

$$\begin{aligned} \int_N^\infty (A_C f + B_C f) x \, dx &= \int_N^\infty \left( -a(x)f(x) + \int_x^\infty a(y)b(x|y)f(y) \, dy \right) x \, dx \\ &= - \int_N^\infty a(x)f(x)x \, dx + \int_N^\infty \left( \int_x^\infty a(y)b(x|y)f(y) \, dy \right) x \, dx \\ &= - \int_N^\infty a(x)f(x)x \, dx + \int_N^\infty a(y)f(y) \left( \int_N^y x b(x|y) \, dx \right) dy \\ &= - \int_N^\infty \left( x - \int_N^x y b(y|x) \, dy \right) a(x)f(x) \, dx =: -c(f) \leq 0. \end{aligned}$$

We have introduced the notation  $c$  to represent the final integral expression, and this functional will have significance in the analysis which follows. The non-negativity of  $c$  comes as a result of the earlier statement regarding  $\int_N^x y b(y|x) \, dy \leq x$ . The conditions of Theorem 2.5.22 have been shown to hold in our case; hence there exists an extension  $(K, D(K))$  of  $(A_C + B_C, D(A_C))$ , which generates a substochastic semigroup  $(G_K(t))_{t \geq 0}$ .  $\square$

This theorem proves only the existence of a generating extension  $K$ , and offers no indication of how exactly  $K$  relates to  $A_C + B_C$ . The nature of the generator  $K$  is closely related to the concept of the honesty of the semigroup (Definition 2.5.24)

and in turn the occurrence of ‘shattering’. This relationship is discussed in [9], where a range of possibilities for  $K$  are considered and it is shown that the cases in which shattering occurs coincide with those in which the semigroup generated by  $K$  is dishonest.

In order to establish the honesty of the semigroup  $(G_K(t))_{t \geq 0}$ , we follow a similar approach to that taken in [10, Section 6.3]. Let us denote by  $\mathbf{E}$  the set of all measurable functions defined on  $(N, \infty)$ , which take values within the extended reals. By  $\mathbf{E}_f$  we denote the subspace of  $\mathbf{E}$  consisting of functions which are finite almost everywhere. We also introduce the set  $\mathbf{F} \subset \mathbf{E}$ , defined as follows. The function  $f \in \mathbf{F}$ , if and only if given a non-negative, non-decreasing sequence  $\{f_n\}_{n=1}^\infty \subset \mathbf{E}$ , where  $\sup_{n \in \mathbb{N}} f_n = |f|$ , we have  $\sup_{n \in \mathbb{N}} (I - A_C)^{-1} f_n \in X_C$ .

Additionally, we place the following two requirements on the operator  $B_C$  and its domain  $D(B_C)$ . Firstly

$$f \in D(B_C) \text{ if and only if } f_+, f_- \in D(B_C), \quad (3.8)$$

where  $f_+ = \max\{f, 0\}$  and  $f_- = -\min\{f, 0\}$ . Secondly, for any two non-decreasing sequences  $\{f_n\}_{n=1}^\infty$  and  $\{g_n\}_{n=1}^\infty$  in  $D(B_C)_+$ , we have that

$$\sup_{n \in \mathbb{N}} f_n = \sup_{n \in \mathbb{N}} g_n \text{ implies } \sup_{n \in \mathbb{N}} B_C f_n = \sup_{n \in \mathbb{N}} B_C g_n. \quad (3.9)$$

**Lemma 3.2.3.** *With  $B_C$  restricted to  $D(A_C)$ ,  $(B_C, D(A_C))$  satisfies the conditions (3.8) and (3.9).*

*Proof.* Initially let us assume that both  $f_+, f_- \in D(A_C)$ . Then, writing  $f$  as  $f = f_+ - f_-$  and using the linearity of  $A$  with the triangle inequality, we get that

$$\|A_C f\|_{X_C} = \|A_C f_+ - A_C f_-\|_{X_C} \leq \|A_C f_+\|_{X_C} + \|A_C f_-\|_{X_C}.$$

Therefore  $f \in D(A_C)$  when  $f_+, f_- \in D(A_C)$ . Now conversely, suppose that  $f \in D(A_C)$ . Since  $0 \leq f_\pm \leq |f|$ , we have

$$\|A_C f_\pm\|_{X_C} = \int_N a(y) f_\pm(y) y \, dy \leq \int_N a(y) |f(y)| y \, dy = \|A_C f\|_{X_C}.$$

Hence if  $f \in D(A_C)$  then  $f_+, f_- \in D(A_C)$ . Taken together, these two results give us the first of our conditions (3.8). The second condition, (3.9), follows using Lebesgue’s monotone convergence theorem, which gives us

$$\sup_{n \in \mathbb{N}} B_C f_n = \mathcal{B} \sup_{n \in \mathbb{N}} f_n = \mathcal{B} \sup_{n \in \mathbb{N}} g_n = \sup_{n \in \mathbb{N}} B_C g_n.$$

Therefore the operator  $B_C$  satisfies both of our requirements when it is restricted to the domain  $D(A_C)$ , which from now on we shall assume unless otherwise stated.  $\square$

We are nearly in a position to demonstrate the honesty of the semigroup  $(G_K(t))_{t \geq 0}$ . However, before we can do so we are required to introduce some further notation and detail a result we had been holding off since the previous chapter.

In addition to the above defined sets, we also introduce  $\mathbf{G} \subset \mathbf{E}$  as the set of all functions  $f \in X_C$  such that if  $\{f_n\}_{n=1}^\infty$  is a non-decreasing sequence of non-negative functions in  $D(A_C)$  such that  $\sup_{n \in \mathbb{N}} f_n = |f|$ , then  $\sup_{n \in \mathbb{N}} B_C f_n < \infty$  almost everywhere.

The final items of notation which we must introduce are the mappings  $\mathbf{B} : D(\mathbf{B})_+ \rightarrow \mathbf{E}_{f,+}$ , where  $D(\mathbf{B}) = \mathbf{G}$  and  $\mathbf{L} : \mathbf{F}_+ \rightarrow X_{C,+}$  defined by

$$\begin{aligned} \mathbf{B}f &:= \sup_{n \in \mathbb{N}} B_C f_n, & f \in D(\mathbf{B})_+, \\ \mathbf{L}f &:= \sup_{n \in \mathbb{N}} R(1, A_C) f_n, & f \in \mathbf{F}_+, \end{aligned}$$

where  $0 \leq f_n \leq f_{n+1}$  for all  $n \in \mathbb{N}$  and  $\sup_{n \in \mathbb{N}} f_n = f$ .

With the set notations and extension operators defined, we can now detail the key generator characterisation result, which will enable us to establish the honesty of our semigroup.

**Theorem 3.2.4.** *If for all  $f \in \mathbf{F}_+$  such that  $-f + \mathbf{B}\mathbf{L}f \in X_C$  and  $c(\mathbf{L}f)$  exists it is true that*

$$\int_N^\infty \mathbf{L}f x \, dx + \int_N^\infty (-f + \mathbf{B}\mathbf{L}f) x \, dx \geq -c(\mathbf{L}f), \quad (3.10)$$

then  $K = \overline{A_C + B_C}$ .

*Proof.* See [10, Theorem 6.22]. □

**Theorem 3.2.5.** *If the fragmentation rate,  $a(x)$ , is such that*

$$\limsup_{x \rightarrow N^+} a(x) < \infty \quad \text{and} \quad a \in L_{\infty, \text{loc}}(N, \infty),$$

then the semigroup  $(G_K(t))_{t \geq 0}$  is honest.

*Proof.* The proof of this result follows closely that of [10, Theorem 8.5]. Since  $A_C f = -af$ , as in [8, Corollary 3.1], we have that  $\mathbf{F} = \{f \in \mathbf{E} : (1+a)^{-1}f \in X_C\}$  and  $\mathbf{L}f = (1+a)^{-1}f$ , whilst by Lebesgue's monotone convergence theorem the operator  $\mathbf{B}$  is given by the integral expression  $\mathcal{B}$ .

For  $f \in \mathbf{F}_+$ , let  $g = \mathbf{L}f = (1+a)^{-1}f \in X_{C,+}$ . Then we see that the condition (3.10) is satisfied if for all  $g \in X_{C,+}$  such that  $-ag + \mathcal{B}g \in X_C$  and  $c(g)$  exists, we have:

$$\int_N^\infty (-a(x)g(x) + (\mathcal{B}g)(x)) x \, dx \geq -c(g). \quad (3.11)$$

By our assumptions regarding the function  $a$ , we have  $ag \in L_1((N, R], x dx)$  for any  $N < R < \infty$  with  $\mathcal{B}g \in L_1((N, R], x dx)$  also, since  $-ag + \mathcal{B}g \in X_C$ . We may write the left-hand side of (3.11) as

$$\begin{aligned} & \int_N^\infty (-a(x)g(x) + (\mathcal{B}g)(x)) x dx = \lim_{R \rightarrow \infty} \int_N^R (-a(x)g(x) + (\mathcal{B}g)(x)) x dx \\ & = \lim_{R \rightarrow \infty} \left\{ - \int_N^R a(x)g(x)x dx + \int_N^R \left( \int_x^\infty a(y)b(x|y)g(y) dy \right) x dx \right\}. \end{aligned} \quad (3.12)$$

If we take the second term from above, split the inner integral in two and then change the order of integration for the integral over the bounded domain, then we get

$$\begin{aligned} & \int_N^R \left( \int_x^\infty a(y)b(x|y)g(y) dy \right) x dx \\ & = \int_N^R \left( \int_x^R a(y)b(x|y)g(y) dy \right) x dx + \int_N^R \left( \int_R^\infty a(y)b(x|y)g(y) dy \right) x dx \\ & = \int_N^R a(y)g(y) \left( \int_N^y xb(x|y) dx \right) dy + \int_N^R \left( \int_R^\infty a(y)b(x|y)g(y) dy \right) x dx. \end{aligned}$$

Substituting this back into (3.12) then yields

$$\begin{aligned} & \int_N^\infty (-a(x)g(x) + (\mathcal{B}g)(x)) x dx \\ & = - \lim_{R \rightarrow \infty} \int_N^R \left( x - \int_N^x yb(y|x) dy \right) a(x)g(x) dx \\ & \quad + \lim_{R \rightarrow \infty} \int_N^R \left( \int_R^\infty a(y)b(x|y)g(y) dy \right) x dx \\ & = -c(g) + \lim_{R \rightarrow \infty} \int_N^R \left( \int_R^\infty a(y)b(x|y)g(y) dy \right) x dx. \end{aligned}$$

The non-negativity of the additional term accompanying  $-c(g)$  gives us (3.11), and with that the honesty of the semigroup  $(G_K(t))_{t \geq 0}$ .  $\square$

Having obtained an  $X_C$ -valued solution to our abstract Cauchy problem equation (3.7), we now examine whether this provides a scalar-valued solution to our original continuous regime equation (3.1). But first we require the following result, which we have delayed until now as it concerns the extended operators introduced above.

**Lemma 3.2.6.** *Suppose that  $(A_C, D(A_C))$  and  $(B_C, D(B_C))$  satisfy the conditions of Theorem 2.5.22 along with conditions (3.8) and (3.9). Additionally let us define the operator  $\mathsf{T}$  with  $D(\mathsf{T}) = \mathsf{LF} \subset X_C$  by*

$$\mathsf{T}u = u - \mathsf{L}^{-1}u,$$

*which is permitted since  $\mathsf{L}$  is one-to-one [10, Theorem 6.18]. Then, the extension  $K$  of  $A_C + B_C$  that generates a substochastic semigroup on  $X_C$  is given by*

$$Ku = \mathsf{T}u + \mathsf{B}u,$$

*with*

$$D(K) = \left\{ u \in D(\mathsf{T}) \cap D(\mathsf{B}) : \mathsf{T}u + \mathsf{B}u \in X_C, \text{ and } \lim_{n \rightarrow \infty} \|(\mathsf{LB})^n u\| = 0 \right\}.$$

*Proof.* See [10, Theorem 6.20] □

**Theorem 3.2.7.** *There exists a measurable scalar-valued representation  $u_C(x, t)$  of the semigroup solution  $(G_K(t)c_0)(x)$ , such that  $u_C(x, t)$  is absolutely continuous with respect to  $t$ , the partial derivative  $\partial_t u_C(x, t)$  exists almost everywhere on  $(N, \infty) \times (0, \infty)$  and  $u_C(x, t)$  satisfies equation (3.1) for almost all  $x > N$  and  $t > 0$ . Further, this representation is unique up to sets of measure zero.*

*Proof.* By Theorem 2.2.15, since  $G_K(t)c_0$  is continuously differentiable, there exists a real-valued function  $u_C(x, t)$ , measurable on  $(N, \infty) \times [0, \infty)$ , which is absolutely continuous with respect to  $t$  for almost all  $x \in (N, \infty)$  and such that  $\partial_t u_C$  exists with

$$\frac{\partial u_C(x, t)}{\partial t} = \left[ \frac{d}{dt} G_K(t)c_0 \right] (x), \quad (3.13)$$

for almost all  $t \in [0, \infty)$  and  $x \in (N, \infty)$ . As stated in Theorems 2.2.14 and 2.2.15, the representation is unique up to sets of measure zero. We noted in Theorem 3.2.5 that the operator  $\mathsf{L}$  is defined by

$$[\mathsf{L}f](x) = (1 + a(x))^{-1}f(x).$$

Hence the operator  $\mathsf{T}$  introduced in Lemma 3.2.6 is given here by

$$[\mathsf{T}f](x) = f(x) - [\mathsf{L}^{-1}f](x) = f(x) - (1 + a(x))f(x) = -a(x)f(x), \quad (3.14)$$

and therefore  $\mathsf{T} \subset \mathcal{A}$ . We have already stated in Theorem 3.2.5 that the operator  $\mathsf{B}$  is given by the integral expression  $\mathcal{B}$ . Hence Lemma 3.2.6 yields

$$K \subset \mathcal{A} + \mathcal{B}.$$

Therefore, the semigroup solution  $G_K(t)c_0$  satisfies

$$\left[ \frac{d}{dt} G_K(t)c_0 \right] (x) = [AG_K(t)c_0] (x) + [BG_K(t)c_0] (x). \quad (3.15)$$

The right-hand side of (3.15) is independent of our choice of representation of  $G_K(t)c_0$ , up to sets of measure zero. Hence combining (3.13) and (3.15), we get that  $u_C(x, t)$  satisfies

$$\frac{\partial u_C(x, t)}{\partial t} = -a(x)u_C(x, t) + \int_x^\infty a(y)b(x|y)u_C(y, t) dy, \quad (3.16)$$

for almost all  $x > N$  and  $t > 0$ , as required.  $\square$

### 3.3 Discrete Fragmentation Regime

We now turn our attention to the discrete mass regime and equation (3.2). As with equation (3.1), our intention is to recast the equations as an abstract differential equation within an appropriate vector space. With this aim in mind, we introduce the space  $X_D = \mathbb{R}^N$ , equipped with the weighted norm:

$$\|v\|_{X_D} = \sum_{j=1}^N j|v_j|, \quad \text{where } v = (v_1, \dots, v_N).$$

The choice of this norm is driven by the fact that, when applied to our solution, it will provide a measure of the total mass within the discrete regime. From the first two terms on the right-hand side of equation (3.2) we get the operators  $A_D$  and  $B_D$  defined on  $X_D$ , elementwise, by

$$(A_D v)_i = -a_i v_i \quad \text{and} \quad (B_D v)_i = \sum_{j=i+1}^N a_j b_{i,j} v_j, \quad \text{for } i = 1, \dots, N,$$

where in the case of  $i = N$ , the empty sum in  $(B_D v)_N$  is taken to be 0. As linear operators on a finite-dimensional space, both  $A_D$  and  $B_D$  are bounded, hence by Theorem 2.4.7,  $A_D + B_D$  generates a uniformly continuous semigroup  $(T(t))_{t \geq 0}$  on  $X_D$ .

**Lemma 3.3.1.** *The semigroup  $(T(t))_{t \geq 0}$  generated by  $A_D + B_D$  on  $X_D$  is a positive semigroup.*

*Proof.* Let us consider the equation

$$(\lambda I_D - (A_D + B_D)) v = w,$$

with  $\lambda > 0$ . Adopting the convention that sums over empty index sets are zero, the above equation written elementwise becomes

$$(\lambda + a_i)v_i - \sum_{j=i+1}^N a_j b_{i,j} v_j = w_i.$$

Inverting this for  $i = N$  we get

$$(\lambda + a_N)v_N = w_N \Rightarrow v_N = \frac{w_N}{\lambda + a_N}.$$

Now suppose that for  $i = N, N-1, \dots, k+1$ , we have  $v_i = F_i(\lambda, w)$  where  $F_i \geq 0$  for  $\lambda > 0$  and  $w \in \mathbb{R}_+^N$ . Then, for  $i = k$ , we have

$$(\lambda + a_k)v_k - \sum_{j=k+1}^N a_j b_{k,j} F_j(\lambda, w) = w_k,$$

and therefore

$$v_k = \frac{1}{\lambda + a_k} \left( w_k + \sum_{j=k+1}^N a_j b_{k,j} F_j(\lambda, w) \right) = F_k(\lambda, w) \geq 0.$$

Therefore, by induction the resolvent operator  $R(\lambda, A_D + B_D)$  is a positive operator for  $\lambda > 0$ . Hence by Theorem 2.4.23 the semigroup  $(T(t))_{t \geq 0}$  is positive.  $\square$

From the third term of equation (3.2) we define the operator  $C : D(C) \subseteq X_C \rightarrow X_D$ , componentwise by

$$(Cf)_i = \int_N^\infty a(y) b_i(y) f(y) dy, \quad D(C) = \{f \in X_C : Cf \in X_D\},$$

for  $i = 1, \dots, N$ . Equation (3.2) is then reformulated as the abstract equation:

$$\frac{d}{dt} u_D(t) = (A_D + B_D)[u_D(t)] + C[u_C(t)], \quad t > 0; \quad u_D(0) = d_0. \quad (3.17)$$

Having introduced the operator  $C$ , we now spend some time examining it in more detail and establishing the properties we will require in the upcoming section. We begin with the following lemma relating the domain of  $C$  with that of  $A_C$  from the previous section.

**Lemma 3.3.2.** For  $f \in D(A_C)$ ,  $\|Cf\|_{X_D} \leq \|A_C f\|_{X_C}$ . Hence  $D(A_C) \subseteq D(C)$ .

*Proof.* Let  $f \in D(A_C)$ . Then

$$\begin{aligned}
\|Cf\|_{X_D} &= \sum_{i=1}^N i \left| \int_N^\infty a(y) b_i(y) f(y) \, dy \right| \\
&\leq \sum_{i=1}^N i \left( \int_N^\infty a(y) b_i(y) |f(y)| \, dy \right) \\
&= \int_N^\infty a(y) |f(y)| \left( \sum_{i=1}^N i b_i(y) \right) \, dy \\
&\leq \int_N^\infty a(y) |f(y)| y \, dy = \|A_C f\|_{X_C}.
\end{aligned} \tag{3.18}$$

The final inequality is a consequence of the mass conservation condition (3.3).  $\square$

Having established that  $C$  is well-defined on  $D(A_C)$ , the next lemma provides a bound on  $\|Cf\|_{X_D}$  when  $f \in D(A_C)$ .

**Lemma 3.3.3.** The operator  $C$  is  $(A_C + B_C)$ -bounded on  $D(A_C)$ .

*Proof.* Combining (3.6) and (3.18), for  $f \in D(A_C)$  we have

$$\begin{aligned}
\|B_C f\|_{X_C} + \|Cf\|_{X_D} &\leq \int_N^\infty a(y) |f(y)| \left( \int_N^y x b(x|y) \, dx \right) \, dy \\
&\quad + \int_N^\infty a(y) |f(y)| \left( \sum_{i=1}^N i b_i(y) \right) \, dy \\
&= \int_N^\infty a(y) |f(y)| \left( \int_N^y x b(x|y) \, dx + \sum_{i=1}^N i b_i(y) \right) \, dy \\
&= \int_N^\infty a(y) |f(y)| y \, dy = \|A_C f\|_{X_C}.
\end{aligned}$$

Subtracting  $\|B_C f\|_{X_C}$  from both sides gives us

$$\begin{aligned}
\|Cf\|_{X_D} &\leq \|A_C f\|_{X_C} - \|B_C f\|_{X_C} = \|A_C f\|_{X_C} - \| -B_C f \|_{X_C} \\
&\leq \|A_C f - (-B_C f)\|_{X_C} = \|(A_C + B_C) f\|_{X_C}.
\end{aligned} \tag{3.19}$$

$\square$

**Lemma 3.3.4.** The operator  $C$  can be extended to  $D(K)$ , with this extension being  $K$ -bounded on  $D(K)$ .

*Proof.* Let  $v \in D(K)$ ; then from Definition 2.3.7, since  $(K, D(K))$  is the closure of  $(A_C + B_C, D(A_C))$ , there exists a sequence  $\{v_n\}_{n=1}^\infty \subset D(A_C)$  such that  $v_n \rightarrow v$  and  $(A_C + B_C)v_n \rightarrow Kv$  in  $X_C$ . By the linearity of the operators and Lemma 3.3.3, we have that

$$\|Cv_m - Cv_n\|_{X_D} \leq \|(A_C + B_C)v_m - (A_C + B_C)v_n\|_{X_C}.$$

The sequence  $\{(A_C + B_C)v_n\}_{n=1}^\infty$  is convergent in  $X_C$ ; therefore it must also be a Cauchy sequence in  $X_C$  and, by the above bound,  $\{Cv_n\}_{n=1}^\infty$  must also be Cauchy in  $X_D$ . Since the space  $X_D$  is complete, the sequence  $\{Cv_n\}_{n=1}^\infty$  must necessarily converge to a limit, which we denote by  $Cv$ . Further, the limit  $Cv$  is independent of the sequence  $\{v_n\}_{n=1}^\infty$ , as we will now demonstrate. Suppose that  $\{w_n\}_{n=1}^\infty \subset D(A_C)$  shares the attributes of  $\{v_n\}_{n=1}^\infty$ ; then we can write

$$\begin{aligned} \|Cw_n - Cv\|_{X_D} &\leq \|Cw_n - Cv_n\|_{X_D} + \|Cv_n - Cv\|_{X_D} \\ &\leq \|(A_C + B_C)w_n - (A_C + B_C)v_n\|_{X_C} + \|Cv_n - Cv\|_{X_D} \\ &\leq \|(A_C + B_C)w_n - Kv\|_{X_C} + \|Kv - (A_C + B_C)v_n\|_{X_C} + \|Cv_n - Cv\|_{X_D}. \end{aligned}$$

From this we may deduce that  $\{Cw_n\}_{n=1}^\infty$  also converges to  $Cv$ . The  $K$ -boundedness of  $C$  on  $D(K)$  is obtained from the  $(A_C + B_C)$ -boundedness of  $C$  by passing the limits through the norms in (3.19).  $\square$

### 3.4 Full System

Having considered both of the regimes separately, we now combine the equations from the continuous regime (3.7) and the discrete regime (3.17), writing them as the following abstract Cauchy problem on the product space  $X = X_D \times X_C$ :

$$\frac{d}{dt}u(t) = \mathbf{A}[u(t)], \quad t > 0; \quad u(0) = u_0 \in D(\mathbf{A}) = X_D \times D(K), \quad (3.20)$$

where  $u(t)$ ,  $\mathbf{A}$  and  $u_0$  are given by

$$u(t) = \begin{pmatrix} u_D(t) \\ u_C(t) \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} (A_D + B_D) & C \\ 0_{DC} & K \end{pmatrix}, \quad u_0 = \begin{pmatrix} d_0 \\ c_0 \end{pmatrix}.$$

The presence of the subscripts on the zero operators indicate the spaces they map from and to; for example,  $0_{DC}$  maps from  $X_D$  into  $X_C$ . Our task is now to prove that the operator  $\mathbf{A}$  generates a semigroup on the space  $X$ . In order to more easily show this, we consider  $(\mathbf{A}, D(\mathbf{A}))$  as the sum of two operators  $(\mathbf{A}_1, D(\mathbf{A}))$  and  $(\mathbf{A}_2, D(\mathbf{A}))$ , where

$$\mathbf{A} = \underbrace{\begin{pmatrix} 0_{DD} & C \\ 0_{DC} & K \end{pmatrix}}_{\mathbf{A}_1} + \underbrace{\begin{pmatrix} (A_D + B_D) & 0_{CD} \\ 0_{DC} & 0_{CC} \end{pmatrix}}_{\mathbf{A}_2}.$$

From the boundedness of  $(A_D + B_D)$  it is easily seen that  $(\mathbf{A}_2, D(\mathbf{A}))$  is a bounded operator. The strategy is then to show that  $(\mathbf{A}_1, D(\mathbf{A}))$  generates a semigroup and then treat  $\mathbf{A}_2$  as a bounded perturbation of this generator. The first of these steps is tackled in the following theorem.

**Theorem 3.4.1.** *The operator  $\mathbf{A}_1$ , as given above, generates a  $C_0$ -semigroup on the product space  $X = X_D \times X_C$ .*

*Proof.* In order to establish that  $\mathbf{A}_1$  is a generator, we demonstrate that the conditions of Theorem 2.5.29 are satisfied by our operator. Conditions (i) to (iii) of Theorem 2.5.29 are either straightforward, or else have already been verified. The element  $0_{DD}$  generates the identity semigroup on  $X_D$ , whilst  $K$  is the generator of the substochastic semigroup  $(G_K(t))_{t \geq 0}$ , as was shown in Theorem 3.2.2. Additionally, the operator  $C$  is  $K$ -bounded on  $D(K)$  as was shown in Lemma 3.3.4.

Condition (iv) requires that  $(\mathbf{A}_1, D(\mathbf{A}))$  be a closed operator. To see this, let us write  $(\mathbf{A}_1, D(\mathbf{A}))$  as

$$\mathbf{A}_1 = \underbrace{\begin{pmatrix} 0_{DD} & 0_{CD} \\ 0_{DC} & K \end{pmatrix}}_{\mathbf{K}} + \underbrace{\begin{pmatrix} 0_{DD} & C \\ 0_{DC} & 0_{CC} \end{pmatrix}}_{\mathbf{C}},$$

with both  $\mathbf{K}$  and  $\mathbf{C}$  having domain  $D(\mathbf{A})$ . Since  $(K, D(K))$  is the generator of a strongly continuous semigroup, by Theorem 2.4.12 it must be a closed operator. It is not difficult to deduce from this that  $(\mathbf{K}, D(\mathbf{A}))$  must also be closed.

Let us now introduce a new norm on the space  $X$ , defined for  $f = \begin{pmatrix} f_D \\ f_C \end{pmatrix} \in X$  by  $\|f\|_\alpha = \alpha \|f_D\|_{X_D} + \|f_C\|_{X_C}$ , where  $0 < \alpha < 1$ . It is a straightforward exercise to show that this new norm is equivalent to the standard norm on  $X$ , and therefore  $(\mathbf{K}, D(\mathbf{A}))$  is closed with respect to this new norm. The  $K$ -boundedness of  $C$  from Lemma 3.3.4 gives us

$$\|\mathbf{C}f\|_\alpha = \alpha \|Cf_C\|_{X_D} \leq \alpha \|Kf_C\|_{X_C} = \alpha \|\mathbf{K}f\|_\alpha.$$

Therefore, with respect to this norm,  $\mathbf{C}$  is  $\mathbf{K}$ -bounded with  $\mathbf{K}$ -bound less than 1. We may then deduce from Lemma 3.3.4, that the operator  $(\mathbf{A}_1, D(\mathbf{A}))$  is closed with respect to the norm  $\|\cdot\|_\alpha$  and as a result of their equivalence, is also closed under the standard norm on  $X$ .

To prove the final condition of Theorem 2.5.29, we introduce the mapping  $\tilde{Q}(t) : D(K) \subseteq X_C \rightarrow X_D$  defined by  $\tilde{Q}(t)f = \int_0^t CG_K(s)f ds$ . For  $f \in D(K)$  we may

write this as

$$\begin{aligned}
\tilde{Q}(t)f &= \int_0^t CG_K(s)f \, ds \\
&= \int_0^t C(\lambda I_C - K)^{-1}(\lambda I_C - K)G_K(s)f \, ds \quad (\lambda > 0) \\
&= C(\lambda I_C - K)^{-1} \int_0^t (\lambda I_C - K)G_K(s)f \, ds \\
&= C(\lambda I_C - K)^{-1} \left\{ \lambda \int_0^t G_K(s)f \, ds - \int_0^t KG_K(s)f \, ds \right\} \\
&= C(\lambda I_C - K)^{-1} \left\{ \lambda \int_0^t G_K(s)f \, ds - \int_0^t G_K(s)Kf \, ds \right\} \\
&= C(\lambda I_C - K)^{-1} \left\{ \lambda \int_0^t G_K(s)f \, ds - G_K(t)f + f \right\}. \tag{3.21}
\end{aligned}$$

The extraction of  $C(\lambda I_C - K)^{-1}$  from within the integral is permitted as it is a bounded linear operator, owing to  $C$  being  $K$ -bounded. The switching of the generator  $K$  and the semigroup operator  $G_K(t)$  is a standard result, detailed in Theorem 2.4.11, whilst, the replacement of the second integral in the final step is a consequence of Lemma 2.4.13. Recalling that  $(G_K(t))_{t \geq 0}$  is a semigroup of contractions, the following norm bound is readily obtained from (3.21):

$$\begin{aligned}
\|\tilde{Q}(t)f\|_{X_D} &\leq \|C(\lambda I_C - K)^{-1}\| \left\{ \lambda \int_0^t \|G_K(s)f\|_{X_C} \, ds + \|G_K(t)f\|_{X_C} + \|f\|_{X_C} \right\} \\
&\leq \|C(\lambda I_C - K)^{-1}\| (\lambda t + 2) \|f\|_{X_C}. \tag{3.22}
\end{aligned}$$

Therefore  $\tilde{Q}(t)$  is bounded on  $D(K)$ . As a densely-defined, bounded linear operator,  $\tilde{Q}(t)$  can be uniquely extended, via taking limits, to a bounded linear operator  $Q(t)$  in  $B(X_C, X_D)$ . Further, by passing limits through the norms, the bound (3.22) holds for all  $u \in X_C$  with  $\tilde{Q}(t)$  replaced by  $Q(t)$ . As such,  $Q(t)$  is uniformly bounded as  $t \searrow 0$ . By Theorem 2.5.29,  $\mathbf{A}_1$  generates a  $C_0$ -semigroup on the product space  $X$ .  $\square$

Having established that  $(\mathbf{A}_1, D(\mathbf{A}_1))$  is a generator, we are now ready to prove the same for the full operator  $(\mathbf{A}, D(\mathbf{A}))$ .

**Theorem 3.4.2.** *The operator  $(\mathbf{A}, D(\mathbf{A}))$ , generates a  $C_0$ -semigroup on  $X = X_D \times X_C$ . Furthermore, this semigroup is given by*

$$\mathbf{T}(t) := \begin{pmatrix} T(t) & R(t) \\ 0_{DC} & G_K(t) \end{pmatrix}, \quad t \geq 0, \tag{3.23}$$

where  $R(t) : X_C \rightarrow X_D$  is the unique bounded linear extension of the operator  $\tilde{R}(t) : D(K) \subseteq X_C \rightarrow X_D$  defined by  $\tilde{R}(t)f = \int_0^t T(t-s)CG_K(s)f \, ds$ .

*Proof.* As the sum of the generator  $(\mathbf{A}_1, D(\mathbf{A}))$  and the bounded linear operator  $(\mathbf{A}_2, D(\mathbf{A}))$ ,  $(\mathbf{A}, D(\mathbf{A}))$  is itself a generator by Theorem 2.5.19. The form of the semigroup comes as a consequence of Theorem 2.5.29.  $\square$

To summarise the results of this chapter so far, the existence of the semigroup  $(\mathbf{T}(t))_{t \geq 0}$ , means that given an initial state  $\binom{d_0}{c_0} \in D(\mathbf{A})$  and provided the conditions of Theorem 3.2.5 are met, namely that the fragmentation rate  $a(x)$  satisfies

$$\limsup_{x \rightarrow N^+} a(x) < \infty \quad \text{and} \quad a \in L_{\infty, \text{loc}}(N, \infty),$$

then there exists a unique solution to the system (3.7) and (3.17). This solution is strongly differentiable with respect to  $t$  and from (3.23), is given by

$$\begin{aligned} u_D(t) &= T(t)d_0 + \int_0^t T(t-s)CG_K(s)c_0 \, ds = T(t)d_0 + \int_0^t T(t-s)Cu_C(s) \, ds, \\ u_C(t) &= G_K(t)c_0. \end{aligned} \tag{3.24}$$

Furthermore, by Theorem 3.2.7, the existence of the semigroup solution  $u_C(t) = G_K(t)c_0$  to (3.7), provides us with a unique (up to sets of measure zero) scalar-valued, classical solution to our original continuous equation (3.1). The nature of the space  $X_D$  and the strong derivative within this space, means that the solution  $u_D(t)$  to (3.17) automatically provides us with a set of unique classical solutions to the equations (3.2). Having determined the existence such solutions, in the upcoming section we establish some key properties displayed by them.

### 3.5 Solution Properties (Non-negativity and Mass Conservation)

The existence of the  $C_0$ -semigroup  $(\mathbf{T}(t))_{t \geq 0}$  provides us with a unique strong solution,  $u(t) = \mathbf{T}(t)u_0$ , to the abstract Cauchy problem (3.20). For the solution to be physically relevant given the problem setting, we would expect it to possess a number of properties. In particular, we hope that the solution preserves non-negativity and demonstrate conservation of mass. First off we establish the non-negativity of the strong solution.

**Lemma 3.5.1.** *Provided that the initial data are non-negative, i.e.  $u_0 = \binom{d_0}{c_0} \in D(\mathbf{A})_+ = X_{D+} \times D(K)_+$ , then the strong solution  $u(t) = \mathbf{T}(t)u_0$ , emanating from  $u_0$ , remains non-negative, that is  $u(t) \in D(\mathbf{A})_+$  for all  $t \geq 0$ .*

*Proof.* Let  $u_0 \in D(\mathbf{A})_+$ . Then the two components of the solution  $u(t)$  are given by (3.24). Since  $(G_K(t))_{t \geq 0}$  is a substochastic semigroup, it preserves non-negativity of the initial datum. Therefore, when  $c_0 \in D(K)_+$  we have  $G_K(t)c_0 \in D(K)_+$

for all  $t \geq 0$ , hence the continuous regime solution satisfies  $u_C(t) \in D(K)_+$  for all  $t \geq 0$ .

As an integral operator with a non-negative kernel, the operator  $C$  is easily seen to be a positive operator. The semigroup  $(T(t))_{t \geq 0}$  is a positive semigroup as was shown in Lemma 3.3.1. Together with the non-negativity of the continuous regime solution, these ensure that the integral term is a non-negative contribution to  $u_D(t)$  whenever  $c_0 \in D(K)_+$ . As stated,  $(T(t))_{t \geq 0}$  is a positive semigroup, and therefore  $u_D(t) \in X_{D+}$  for all  $t \geq 0$  when the initial system state satisfies  $u_0 = \begin{pmatrix} d_0 \\ c_0 \end{pmatrix} \in X_{D+} \times D(K)_+$ .

Together, having  $u_D(t) \in X_{D+}$  and  $u_C(t) \in D(K)_+$  gives us  $u(t) \in D(\mathbf{A})_+$  as required.  $\square$

Let  $u(t) = \begin{pmatrix} u_D(t) \\ u_C(t) \end{pmatrix}$  be the solution to the abstract Cauchy problem (3.20) with non-negative initial data. Then the masses in the discrete and continuous regimes, at time  $t$ , are then given by

$$M_D(t) = \sum_{i=1}^N i u_{D_i}(t) \quad \text{and} \quad M_C(t) = \int_N^\infty (u_C(t))(x) x \, dx,$$

respectively. Summing these gives us the total mass in the system  $M(t) = M_D(t) + M_C(t)$  at time  $t$ . In each fragmentation event, mass is redistributed from larger particles to the smaller resulting particles, but the total mass involved should be conserved. This mass conservation was built into our model in the form of the conditions (3.3) and (3.4). Therefore, although  $M_D(t)$  may increase and  $M_C(t)$  decrease as larger particles break into smaller pieces, we would expect the total mass,  $M(t)$ , to remain constant.

**Lemma 3.5.2.** *The total mass within the system is conserved, that is  $M(t)$  remains constant for all  $t \geq 0$ .*

*Proof.* Since  $(G_K(t))_{t \geq 0}$  is an honest semigroup, by Definition 2.5.24 we have

$$\begin{aligned} \frac{d}{dt} M_C(t) &= \frac{d}{dt} \int_N^\infty (u_C(t))(x) x \, dx = -c(u_C(t)) \\ &= - \int_N^\infty \left( x - \int_N^x y b(y|x) \, dy \right) a(x) (u_C(t))(x) \, dx. \end{aligned} \quad (3.25)$$

Similarly, for the mass within the discrete regime we have

$$\begin{aligned}
\frac{d}{dt}M_D(t) &= \sum_{i=1}^N i \frac{d}{dt}u_{Di}(t) = \sum_{i=1}^N i ((A_D + B_D)[u_D(t)] + C[u_F(t)])_i \\
&= \sum_{i=1}^N i \left( -a_i u_{Di}(t) + \sum_{j=i+1}^N a_j b_{i,j} u_{Dj}(t) + \int_N^\infty a(y) b_i(y) (u_C(t))(y) dy \right) \\
&= - \sum_{i=2}^N \left( i - \sum_{j=1}^{i-1} j b_{j,i} \right) a_i u_{Di}(t) + \int_N^\infty \left( \sum_{i=1}^N i b_i(y) \right) a(y) (u_C(t))(y) dy \quad (3.26)
\end{aligned}$$

$$= \int_N^\infty \left( \sum_{i=1}^N i b_i(y) \right) a(y) (u_C(t))(y) dy. \quad (3.27)$$

The term  $a_1 u_{D1}(t)$  is dropped from the first summation in going to the third line since  $a_1 = 0$ . In the final step, the loss of the first term is a consequence of condition (3.4). The rate of change of the total mass  $M(t)$  is given by the addition of (3.25) and (3.27), which by (3.3) yields

$$\begin{aligned}
\frac{d}{dt}M(t) &= - \int_N^\infty \left( x - \int_N^x y b(y|x) dy \right) a(x) (u_C(t))(x) dx \\
&\quad + \int_N^\infty \left( \sum_{i=1}^N i b_i(x) \right) a(x) (u_C(t))(x) dx \\
&= - \int_N^\infty \left( x - \int_N^x y b(y|x) dy - \sum_{i=1}^N i b_i(x) \right) a(x) (u_C(t))(x) dx \quad (3.28) \\
&= 0,
\end{aligned}$$

thus confirming that  $M(t)$  remains constant for all  $t \geq 0$ , and so mass is conserved.  $\square$

In this chapter we introduced our mixed discrete–continuous fragmentation model (3.1) and (3.2). Utilising the theory of operator semigroups, we proved the existence of a unique, strong solution to our system within the setting of the appropriate Banach space. In turn, this enabled us to establish the existence of a unique classical solution to our equations. Finally, we showed that these solutions preserved non-negativity and conserved mass, two properties we would expect from a physically relevant solution. Considering the difficulties discussed in Chapter 1, concerning obtaining analytic solutions to such equations, in the following chapter we look to develop a numerical scheme for the approximate solution of equations (3.1) and (3.2).

# Chapter 4

## Numerical Approximation for a Mixed Discrete–Continuous Fragmentation Model

### 4.1 Introduction

Most of the equations introduced in Chapter 1 can only be solved analytically for a limited number of specific cases. Therefore we often have to resort to approximate solutions generated by an appropriate numerical scheme. We would expect this also to be the case for our mixed discrete–continuous model. In this section we present a numerical scheme for the solution of the mixed fragmentation model given by equations (3.1) and (3.2). The basis of the scheme is a finite volume discretisation of the continuous regime equation (3.1). Finite volume schemes have been commonly applied to the solution of coagulation and fragmentation equations. For example, in the article [16], such a scheme is used in the case of the binary coagulation and fragmentation equation (1.4), whilst in [44] we see this method utilised in the solution of the standard multiple fragmentation equation (1.5).

When considering the numerical solution of our equations, we encounter an issue in that the range of the continuous mass variable  $x$  is an unbounded interval, which presents a computational problem. We therefore introduce a truncation parameter  $R > N$ , and restrict the continuous mass variable to the range  $N < x < R$ . Therefore, in place of equation (3.1), we consider the truncated version

$$\begin{aligned} \frac{\partial u_C^R(x, t)}{\partial t} &= -a(x)u_C^R(x, t) + \int_x^R a(y)b(x|y)u_C^R(y, t) dy, \quad N < x < R, \quad t > 0, \quad (4.1) \\ u_C^R(x, 0) &= \chi_{(N, R)}(x)c_0(x), \quad N < x < R, \end{aligned}$$

where  $\chi_{(N,R)}$  denotes the characteristic function of the interval  $(N, R)$ . Taking our lead from the aforementioned articles, we now rewrite equation (4.1) in a conservative form, although in our case we must include an additional sink term to account for the mass leaked down to the discrete regime. Therefore we end up with the following equation for the mass quantity  $xu_C^R(x, t)$ :

$$\frac{\partial (xu_C^R)}{\partial t} = \frac{\partial \mathcal{F}^R (xu_C^R)}{\partial x} - S(xu_C^R), \quad u_C^R(x, 0) = c_0(x), \quad \text{for } N < x < R, \quad t > 0, \quad (4.2)$$

where  $\mathcal{F}^R$  is a truncated flux term, given by

$$\mathcal{F}^R(f) = \int_x^R \int_N^x \frac{y}{z} a(z) b(y|z) f(z) \, dy \, dz, \quad \text{for } N < x < R,$$

and the sink term  $S$  is given by

$$S(f) = \frac{a(x)}{x} \sum_{i=1}^N i b_i(x) f(x), \quad \text{for } x > N.$$

The equation (4.1) may be recovered from (4.2) by an application of Leibniz's rule for differentiating under the integral. The use of Leibniz's rule here is made fully rigorous in Appendix C. Before continuing further, we establish a result concerning the behaviour of the flux term  $\mathcal{F}^R$  at the limits of our domain.

**Lemma 4.1.1.** *If the kernels  $a$  and  $b$  are assumed to belong to  $L_{\infty,loc}[N, \infty)$  and  $L_{\infty,loc}([N, \infty) \times [N, \infty))$  respectively, which will be the case in the upcoming analysis, then for  $f \in L_1(N, R)$ , the flux term  $\mathcal{F}^R(f)$  satisfies*

$$\lim_{x \rightarrow N, R} |\mathcal{F}^R(f)(x)| = 0.$$

*Proof.* It is a straightforward operation to bound  $\mathcal{F}^R(f)$  as follows:

$$|\mathcal{F}^R(f)(x)| \leq \int_N^R \chi_{(x,R)}(z) \frac{a(z) |f(z)|}{z} \left( \int_N^x y b(y|z) \, dy \right) \, dz, \quad (4.3)$$

which holds for  $x \in (N, R)$ . Recalling the mass conservation condition (3.3), we deduce that

$$\chi_{(x,R)}(z) \left( \int_N^x y b(y|z) \, dy \right) \leq \int_N^z y b(y|z) \, dy \leq z,$$

for all  $z \in (N, R)$ . Hence the integrand appearing in (4.3) is bounded above by  $a(z) |f(z)|$ , which, due to  $a \in L_{\infty,loc}[N, \infty)$  and  $f \in L_1(N, R)$ , is integrable.

Considering the limit as  $x \rightarrow N$  first, if we denote by  $\beta(R)$  the essential supremum of  $b$  over  $[N, R] \times [N, R]$ , then we have

$$\chi_{(x,R)}(z) \left( \int_N^x yb(y|z) dy \right) \leq x\beta(R)(x - N).$$

As such, the integrand in (4.3) converges pointwise to 0 over  $z \in (N, R)$  as we let  $x \searrow N$ . An application of the Lebesgue dominated convergence theorem then gives the required convergence of  $|\mathcal{F}^R(f)(x)|$  as  $x \searrow N$ . Turning now to the limit as  $x \nearrow R$ , another application of condition (3.3) provides us with

$$\chi_{(x,R)}(z) \left( \int_N^x yb(y|z) dy \right) \leq \chi_{(x,R)}(z) \int_N^z yb(y|z) dy \leq \chi_{(x,R)}(z)z,$$

for  $z \in (N, R)$ . Therefore, the integrand from (4.3) must again converge pointwise to 0 over  $(N, R)$ , this time as we let  $x \nearrow R$ . Another application of the Lebesgue dominated convergence theorem gives the convergence of  $|\mathcal{F}^R(f)(x)|$  to 0, as  $x \nearrow R$ .  $\square$

This result will be utilised later in a number of results, most significantly in approximating  $\mathcal{F}^R$  within our numerical scheme and in establishing a weak formulation of equation (4.2).

The truncation of the continuous mass interval also has an impact on our discrete regime equation; therefore, instead of equation (3.2), we consider

$$\begin{aligned} \frac{du_{Di}^R(t)}{dt} &= -a_i u_{Di}^R(t) + \sum_{j=i+1}^N a_j b_{i,j} u_{Dj}^R(t) + \int_N^R a(y) b_i(y) u_C^R(y, t) dy, \\ u_{Di}^R(0) &= d_{0i}, \text{ for } i = 1, 2, \dots, N, \quad t > 0. \end{aligned} \quad (4.4)$$

In the case of  $i = N$ , the empty sum above is taken to be zero; this convention will be adopted in all similar cases which follow.

## 4.2 Development of the Numerical Scheme

We now introduce our numerical approximation scheme for the truncated system, (4.2) and (4.4). First we must discretise the continuous mass variable  $x$ , and so we introduce the mesh  $\{x_{i-1/2}\}_{i=0}^{I_h}$  on the interval  $(N, R)$ , with

$$x_{-1/2} = N, \quad x_{I_h-1/2} = R, \quad x_i = (x_{i-1/2} + x_{i+1/2})/2, \quad h/k < \Delta x_i = x_{i+1/2} - x_{i-1/2} < h,$$

where  $h \in (0, 1)$  and  $k > 1$  is some constant. Additionally we denote the interval  $[x_{i-1/2}, x_{i+1/2})$  by  $\Lambda_i$ , however the left-hand most interval  $\Lambda_0$  is taken to be

$(x_{-1/2}, x_{1/2})$ .

For the time variable  $t$ , if  $T$  is the final time up to which we wish to compute an approximate solution, then we define the time step  $\Delta t = T/M$  where  $M$  is some large integer. The time points are then given by  $t_n = n\Delta t$  for  $n = 0, 1, \dots, M$  with corresponding time intervals  $\tau_n = [t_n, t_{n+1})$  for  $n = 0, 1, \dots, M - 1$ .

We restrict the choice of the mesh by assuming the existence of constants  $k_1$  and  $k_2$  so that the mesh sizes  $h$  and  $\Delta t$  satisfy

$$k_1 h \leq \Delta t \leq k_2 h. \quad (4.5)$$

The numerical scheme requires representative values for the functions  $a(x)$ ,  $b(x|y)$  and  $b_i(y)$  over the appropriate intervals. This is done by taking their average value over each interval. Therefore we define

$$A_i = \frac{1}{\Delta x_i} \int_{\Lambda_i} a(x) dx \quad \text{for } i = 0, 1, \dots, I_h - 1,$$

as our approximation for  $a(x)$  over the interval  $\Lambda_i$ . We approximate  $b(x|y)$  over  $\Lambda_i \times \Lambda_j$  by

$$B_{i,j} = \frac{1}{\Delta x_i \Delta x_j} \int_{\Lambda_j} \int_{\Lambda_i} b(x|y) dx dy \quad \text{for } i = 0, 1, \dots, I_h - 1 \text{ and } j = 0, 1, \dots, I_h - 1,$$

and the functions  $b_i(y)$  are approximated over  $\Lambda_j$  by the values

$$\tilde{B}_{i,j} = \frac{1}{\Delta x_j} \int_{\Lambda_j} b_i(y) dy \quad \text{for } i = 1, 2, \dots, N \text{ and } j = 0, 1, \dots, I_h - 1.$$

We note by our previous restrictions on  $a$ ,  $b$  and  $b_i$ , that each of the values introduced above must be non-negative. If  $\chi_I$  denotes the characteristic function of a set  $I$ , then we can construct piecewise constant approximations to the functions  $a$ ,  $b$  and  $b_i$  as follows:

$$a^h(x) = \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) A_i, \quad b^h(x|y) = \sum_{j=0}^{I_h-1} \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \chi_{\Lambda_j}(y) B_{i,j}, \quad b_i^h(y) = \sum_{j=0}^{I_h-1} \chi_{\Lambda_j}(y) \tilde{B}_{i,j}.$$

This is a standard approximation method and assuming the kernels are suitably restricted, the approximations will converge pointwise to the desired functions almost everywhere on the appropriate domains. This convergence will be utilised in the following chapter to establish the weak convergence of our numerically approximated solutions. Therefore we take a short aside to establish this convergence rigorously in the following lemma.

**Lemma 4.2.1.** *If the kernels  $a$  and  $b$  are assumed to be  $L_{\infty,loc}$  on  $[N, \infty)$  and  $[N, \infty) \times [N, \infty)$  respectively, as we shall in the following chapter, then for any fixed  $R > N$ , the approximations  $a^h$ ,  $b^h$  and  $b_i^h$  converge pointwise to  $a$ ,  $b$  and  $b_i$  almost everywhere on the domains  $(N, R)$ ,  $(N, R) \times (N, R)$  and  $(N, R)$  respectively.*

*Proof.* Consider a sequence of partitions of the interval  $(N, R)$  as described in Section 4.2, parameterised by  $h$ . For any such partition we have that

$$\begin{aligned} a^h(x) - a(x) &= \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) A_i - a(x) \\ &= \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) (A_i - a(x)) \\ &= \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \left( \frac{1}{\Delta x_i} \int_{\Lambda_i} a(y) dy - a(x) \right). \end{aligned}$$

Hence, we have the bound

$$|a^h(x) - a(x)| \leq \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \left| \frac{1}{\Delta x_i} \int_{\Lambda_i} a(y) dy - a(x) \right|.$$

Let us denote by  $i_{x,h}$  the non-negative integer for which  $x \in \Lambda_i$  in the partition where the mesh size parameter takes the value  $h$ , so that

$$\begin{aligned} |a^h(x) - a(x)| &\leq \left| \frac{1}{\Delta x_{i_{x,h}}} \int_{\Lambda_{i_{x,h}}} a(y) dy - a(x) \right| \\ &\leq \frac{1}{\Delta x_{i_{x,h}}} \int_{\Lambda_{i_{x,h}}} |a(y) - a(x)| dy. \end{aligned}$$

Let us ‘extend’ the function  $a$  and the approximation  $a^h$  from the interval  $(N, R)$  to the whole of the real-line by zero. Recalling the bounds on our mesh size from Section 4.2, we get  $1/\Delta x_{i_{x,h}} \leq k/h$  and  $\Lambda_{i_{x,h}} \subseteq B(x, h)$ , where  $B(x, h)$  denotes the open ball of radius  $h$  centred at  $x$ . Together these give us

$$\begin{aligned} |a^h(x) - a(x)| &\leq \frac{k}{h} \int_{B(x,h)} |a(y) - a(x)| dy \\ &= 2k \frac{1}{2h} \int_{B(x,h)} |a(y) - a(x)| dy. \end{aligned}$$

Now as  $a \in L_{\infty,loc}([N, \infty))$ , we must have  $a \in L_1([N, R])$  for any choice of  $N < R < \infty$ . The Lebesgue differentiation theorem (Theorem 2.1.4) tells us that almost every point of  $(N, R)$  must be a Lebesgue point of  $a$ , and if we assume that  $x$  is such a point we obtain

$$|a^h(x) - a(x)| \leq 2k \frac{1}{2h} \int_{B(x,h)} |a(y) - a(x)| dy \rightarrow 0,$$

as  $h \searrow 0$ . Therefore  $a^h(x)$  converges pointwise to  $a(x)$ , almost everywhere on  $(N, R)$ .

The above argument can readily be adapted to show that the approximation  $b^h(x|y)$  converges pointwise to  $b(x|y)$  almost everywhere on  $(N, R) \times (N, R)$ . Following the same reasoning we obtain

$$|b^h(x|y) - b(x|y)| \leq \frac{1}{\Delta x_{i_x, h} \Delta x_{j_y, h}} \int_{\Lambda_{i_x, h} \times \Lambda_{j_y, h}} |b^h(u|v) - b(x|y)| \, du \, dv,$$

where  $j_{y, h}$  is the integer such that  $y \in \Lambda_{j_{y, h}}$ . Similarly to  $a$ , we extend the function  $b$  and its approximation  $b^h$  by zero, from  $(N, R) \times (N, R)$  to the whole of  $\mathbb{R}^2$ . Now in  $\mathbb{R}^2$ , the partition element  $\Lambda_{i_x, h} \times \Lambda_{j_y, h}$  is contained within the ball  $B((x, y), h)$  and  $\Delta x_{i_x, h} \Delta x_{j_y, h} \geq h^2/k^2$ , hence

$$\begin{aligned} |b^h(x|y) - b(x|y)| &\leq \frac{k^2}{h^2} \int_{B((x, y), h)} |b^h(u|v) - b(x|y)| \, du \, dv \\ &= 2\pi k^2 \frac{1}{2\pi h^2} \int_{B((x, y), h)} |b^h(u|v) - b(x|y)| \, du \, dv. \end{aligned}$$

The Lebesgue differentiation theorem (Theorem 2.1.4) then gives us that the above bound converges to zero, almost everywhere, as  $h \searrow 0$ . The proof of the convergence of  $a^h$  and  $b^h$  relied on our assumption of them being  $L_{\infty, loc}$ , an assumption that we haven't explicitly made for the functions  $b_i^h$ . However, due to the mass conservation condition (3.3), the functions  $b_i(v)$  must automatically be contained in  $L_{\infty, loc}([N, \infty))$ , as demonstrated here. Condition (3.3) gives us

$$\sum_{i=1}^N i b_i(y) = y - \int_N^y x b(x|y) \, dx \leq y \Rightarrow b_i(y) \leq y, \quad \text{for } i = 1, \dots, N. \quad (4.6)$$

By the Heine–Borel theorem, in  $\mathbb{R}$  the compact sets and those which are closed and bounded are one and the same, hence each  $b_i(y)$  must be bounded on any compact set.

By the same argument as we applied to  $a^h$ , each of the approximations  $b_i^h(y)$  must converge pointwise to the respective  $b_i(y)$  almost everywhere on  $(N, R)$  as  $h \searrow 0$ .  $\square$

We are now ready to construct the approximation scheme. Let  $u_C^{n, i}$  denote our approximation to  $u_C^R(x, t)$  over the mass interval  $\Lambda_i$  for the time interval  $\tau_n$ . The equation (4.2) is then approximated by

$$x_i \frac{u_C^{n+1, i} - u_C^{n, i}}{\Delta t} = \frac{F_{i+1/2}^n - F_{i-1/2}^n}{\Delta x_i} - S_i^n,$$

where  $F_{i-1/2}^n$  is an approximation of the flux  $\mathcal{F}^R(xu_C^R)$  at the point  $x = x_{i-1/2}$  in the time interval  $\tau_n$ , and is given by

$$\begin{aligned} (\mathcal{F}^R(xu_C^R))(x_{i-1/2}) &= \int_{x_{i-1/2}}^R \int_N^{x_{i-1/2}} ya(z)b(y|z)u_C^R(z,t) dy dz \\ &= \sum_{j=i}^{I_h-1} \int_{\Lambda_j} \left( \sum_{k=0}^{i-1} \int_{\Lambda_k} ya(z)b(y|z)u_C^R(z,t) dy \right) dz \\ &\approx \sum_{j=i}^{I_h-1} \sum_{k=0}^{i-1} x_k A_j B_{k,j} u_C^{n,j} \Delta x_k \Delta x_j =: F_{i-1/2}^n, \end{aligned}$$

for  $i = 1, \dots, I_h - 1$ , with  $F_{-1/2}^n = F_{I_h-1/2}^n = 0$ , which can be justified by Lemma 4.1.1. The values  $S_i^n$  approximate the sink term  $S(xu_C^R)$  over  $\Lambda_i$  for the time interval  $\tau_n$ , and are computed by

$$S_i^n = A_i \sum_{j=1}^N j \tilde{B}_{j,i} u_C^{n,i} \text{ for } i = 0, 1, \dots, I_h - 1. \quad (4.7)$$

This gives rise to the following numerical method for the generation of the approximations  $u_C^{n,i}$ :

$$u_C^{n+1,i} = u_C^{n,i} + \frac{\Delta t}{x_i \Delta x_i} (F_{i+1/2}^n - F_{i-1/2}^n) - \frac{\Delta t}{x_i} S_i^n \text{ for } i = 0, 1, \dots, I_h - 1. \quad (4.8)$$

The sequence of approximations generated by (4.8) requires us to provide an initial set of values to get started. For our starting values we simply average the initial datum over each of the mass intervals; hence

$$u_C^{0,i} = \frac{1}{\Delta x_i} \int_{\Lambda_i} c_0(x) dx \text{ for } i = 0, 1, \dots, I_h - 1. \quad (4.9)$$

Then our approximation to  $u_C^R(x, t)$  over  $(N, R) \times [0, T)$  is constructed as follows:

$$u_C^h(x, t) = \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \chi_{\tau_n}(t) u_C^{n,i}. \quad (4.10)$$

The convergence proof for our numerical scheme in the following chapter requires the initial approximation given by (4.9) and (4.10) to converge strongly in the appropriate space, which we provide in the following lemma.

**Lemma 4.2.2.** *If the initial mass distribution  $c_0 \in X_C$ , then for any  $R > N$  the associated approximation  $u_C^h(x, 0)$  provided by (4.9) and (4.10) converges strongly in  $L_1(N, R)$  to the restriction of  $c_0$  to  $(N, R)$ .*

*Proof.* Let  $f \in L_1(N, R)$ , and let us approximate it over  $(N, R)$  by introducing the approximation operator  $\mathcal{P}_h$  as follows:

$$(\mathcal{P}_h f)(x) := \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \frac{1}{\Delta x_i} \int_{\Lambda_i} f(y) dy.$$

From the linearity of the integral it can easily be seen that  $\mathcal{P}_h$  is a linear operator. The restriction placed on the mesh size that  $h/k < \Delta x_i$  gives us

$$|(\mathcal{P}_h f)(x)| \leq \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \frac{k}{h} \int_{\Lambda_i} |f(y)| dy,$$

and therefore

$$\begin{aligned} \int_N^R |(\mathcal{P}_h f)(x)| dx &\leq \int_N^R \left( \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \frac{k}{h} \int_{\Lambda_i} |f(y)| dy \right) dx \\ &\leq \sum_{i=0}^{I_h-1} \left( \frac{k}{h} \int_{\Lambda_i} |f(y)| dy \right) \underbrace{\int_N^R \chi_{\Lambda_i}(x) dx}_{=\Delta x_i \leq h} \\ &\leq k \sum_{i=0}^{I_h-1} \int_{\Lambda_i} |f(y)| dy = k \|f\|_{L_1(N,R)}. \end{aligned} \quad (4.11)$$

Hence  $\mathcal{P}_h$  is also bounded on  $L_1(N, R)$ . For the time being let us assume that  $f \in C_c^\infty(N, R)$ . Then, using the fundamental theorem of calculus, we get

$$\begin{aligned} \|\mathcal{P}_h f - f\|_{L_1(N,R)} &= \int_N^R \left| \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \frac{1}{\Delta x_i} \int_{\Lambda_i} f(y) dy - f(x) \right| dx \\ &\leq \int_N^R \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \frac{1}{\Delta x_i} \int_{\Lambda_i} |f(y) - f(x)| dy dx \\ &\leq \frac{k}{h} \int_N^R \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \int_{\Lambda_i} \left| \int_x^y f'(s) ds \right| dy dx \\ &\leq \frac{k}{h} \sum_{i=0}^{I_h-1} \int_{\Lambda_i} \int_{\Lambda_i} \int_x^y |f'(s)| ds dy dx \\ &\leq \frac{k}{h} \sum_{i=0}^{I_h-1} \int_{\Lambda_i} \int_{\Lambda_i} \int_{\Lambda_i} |f'(s)| ds dy dx \\ &\leq \frac{k}{h} \sum_{i=0}^{I_h-1} h^2 \int_{\Lambda_i} |f'(s)| ds = kh \|f'\|_{L_1(N,R)}. \end{aligned} \quad (4.12)$$

Now given  $f \in L_1(N, R)$ , by the density of  $C_c^\infty(N, R)$  in  $L_1(N, R)$  from Lemma 2.1.2, we approximate  $f$  by a sequence  $\{f_j\}_{j=1}^\infty \subset C_c^\infty(N, R)$  such that  $\|f_j - f\|_{L_1(N, R)} \rightarrow 0$  as  $j \rightarrow \infty$ . Then we have

$$\begin{aligned} \|\mathcal{P}_h f - f\|_{L_1(N, R)} &= \|\mathcal{P}_h f - \mathcal{P}_h f_j + \mathcal{P}_h f_j - f_j + f_j - f\|_{L_1(N, R)} \\ &\leq \|\mathcal{P}_h f - \mathcal{P}_h f_j\|_{L_1(N, R)} + \|\mathcal{P}_h f_j - f_j\|_{L_1(N, R)} + \|f_j - f\|_{L_1(N, R)} \\ &\leq k \|f - f_j\|_{L_1(N, R)} + kh \|f'_j\|_{L_1(N, R)} + \|f_j - f\|_{L_1(N, R)}, \end{aligned}$$

where the last line is as a consequence of (4.11) and (4.12). For fixed  $j$ , letting  $h \rightarrow 0$  gives us

$$\lim_{h \rightarrow 0} \|\mathcal{P}_h f - f\|_{L_1(N, R)} \leq (k+1) \|f - f_j\|_{L_1(N, R)}.$$

As the left-hand side is independent of  $j$  we then let  $j \rightarrow \infty$  to obtain

$$\lim_{h \rightarrow 0} \|\mathcal{P}_h f - f\|_{L_1(N, R)} = 0.$$

The result then follows immediately by taking the restriction of  $c_0$  to  $(N, R)$  as our  $f$  and realising that  $u_C^h(x, 0)$  is then given by  $\mathcal{P}_h f$ .  $\square$

Now let  $u_D^{n,i}$  denote our approximation of  $u_{D_i}^R(t)$  over the time interval  $\tau_n$ . Equation (4.4) is then approximated as

$$\frac{u_D^{n+1,i} - u_D^{n,i}}{\Delta t} = -a_i u_D^{n,i} + \sum_{j=i+1}^N a_j b_{i,j} u_D^{n,j} + \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \Delta x_j,$$

giving rise to the relation

$$u_D^{n+1,i} = (1 - \Delta t a_i) u_D^{n,i} + \Delta t \sum_{j=i+1}^N a_j b_{i,j} u_D^{n,j} + \Delta t \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \Delta x_j \quad \text{for } i = 1, \dots, N. \quad (4.13)$$

The starting values for the discrete approximation are simply given by the initial condition vector  $d_0$ , so that  $u_D^{0,i} = d_{0i}$  for  $i = 1, \dots, N$ . Then our approximations  $u_{D_i}^h(t)$  to  $u_{D_i}^R(t)$  for  $t \in [0, T)$  are given by

$$u_{D_i}^h(t) = \sum_{n=0}^{M-1} \chi_{\tau_n}(t) u_D^{n,i} \quad \text{for } i = 1, 2, \dots, N. \quad (4.14)$$

### 4.3 Properties of the Numerical Solutions: Non-negativity and Mass Conservation

In the preceding chapter we proved the existence of a solution to our system (3.1) and (3.2). This solution was shown to possess a number of properties that

we would expect given the physical nature of the model, namely the solution preserved non-negativity and conserved total mass. In the following sections we examine whether the approximate solution provided by (4.10) and (4.14), also displays these properties.

### 4.3.1 Non-negativity of the Numerical Solutions

**Lemma 4.3.1.** *For a fixed partition  $(x_{i-1/2})_{i=0}^{I_h}$ , suppose that  $\Delta t$  is sufficiently small that the following condition is satisfied:*

$$0 < \Delta t \leq \frac{x_i}{A_i \left( \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k + \sum_{j=1}^N j \tilde{B}_{j,i} \right)},$$

for all  $i \in \{0, 1, \dots, I_h - 1\}$  such that the denominator is non-zero, and

$$0 < \Delta t \leq \frac{1}{a_i},$$

for all  $i \in \{2, \dots, N\}$  such that  $a_i \neq 0$ . Then, the approximate solutions defined by (4.10) and (4.14) preserve non-negativity.

*Proof.* Starting with the approximation for the continuous regime, let us consider equation (4.8). By cancelling common terms we get that

$$F_{i+1/2}^n - F_{i-1/2}^n = x_i \Delta x_i \sum_{j=i+1}^{I_h-1} A_j B_{i,j} u_C^{n,j} \Delta x_j - A_i u_C^{n,i} \Delta x_i \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k \quad (4.15)$$

for  $i = 1, \dots, I_h - 2$ . Therefore we have

$$\begin{aligned} & \frac{\Delta t}{x_i \Delta x_i} (F_{i+1/2}^n - F_{i-1/2}^n) - \frac{\Delta t}{x_i} S_i \\ &= \Delta t \sum_{j=i+1}^{I_h-1} A_j B_{i,j} u_C^{n,j} \Delta x_j - \frac{\Delta t}{x_i} A_i u_C^{n,i} \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k - \frac{\Delta t}{x_i} A_i u_C^{n,i} \sum_{j=1}^N j \tilde{B}_{j,i} \\ &= \Delta t \sum_{j=i+1}^{I_h-1} A_j B_{i,j} u_C^{n,j} \Delta x_j - \frac{\Delta t}{x_i} A_i u_C^{n,i} \left( \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k + \sum_{j=1}^N j \tilde{B}_{j,i} \right). \end{aligned}$$

Substituting this into (4.8) gives us

$$u_C^{n+1,i} = \left( 1 - \frac{\Delta t}{x_i} A_i \left( \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k + \sum_{j=1}^N j \tilde{B}_{j,i} \right) \right) u_C^{n,i} + \Delta t \sum_{j=i+1}^{I_h-1} A_j B_{i,j} u_C^{n,j} \Delta x_j,$$

for  $i = 1, \dots, I_h - 2$ . The cases  $i = 0$  and  $i = I_h - 1$  can be handled similarly to

obtain the same result, where the empty sums are taken as 0.

From this it is clear that if each of the approximations  $u_C^{n,i}$  is non-negative, and provided  $\Delta t$  is sufficiently small such that the term within the outer brackets is non-negative, then each of the approximations  $u_C^{n+1,i}$ , for the subsequent time-step, will also be non-negative. Hence to ensure the approximations  $u_C^{n,i}$  remain non-negative we can take

$$0 < \Delta t \leq \frac{x_i}{A_i \left( \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k + \sum_{j=1}^N j \tilde{B}_{j,i} \right)} \quad \text{for } i = 0, 1, \dots, I_h - 1. \quad (4.16)$$

In the case of the denominator being zero, the non-negativity of the  $u_C^{n+1,i}$  can be seen to be automatically satisfied for all values of  $\Delta t$ .

Turning to the approximation for the discrete regime, it is immediately clear from the form of (4.13) that if all of the values  $u_C^{n,i}$  and  $u_D^{n,i}$  are non-negative, then each  $u_D^{n+1,i}$  will be non-negative if for each  $i = 1, \dots, N$  we have that  $1 - \Delta t a_i$  is non-negative. This can be ensured by taking

$$0 < \Delta t \leq \frac{1}{a_i} \quad \text{for } i = 2, \dots, N \text{ such that } a_i \neq 0. \quad (4.17)$$

Therefore if we choose a  $\Delta t$  small enough that both (4.16) and (4.17) are satisfied, then our approximate solutions will remain non-negative.  $\square$

From now on we shall assume that conditions (4.16) and (4.17) are satisfied and that  $c_0(x) \geq 0$  and each  $d_{0i} \geq 0$  so that our approximations remain non-negative.

*Remark 4.3.2.* The bound (4.16) is dependent on the mesh and it is perhaps not immediately apparent how this bounding value might vary as we refine the mesh. In particular, it would be advantageous to confirm that it is indeed possible to find a constant  $k_1$ , such that conditions (4.5) and (4.16) can be satisfied simultaneously, whilst  $h \searrow 0$ . In the following chapter we will place restrictions on the functions  $a$  and  $b$ ; these constraints will allow us to guarantee the existence of such a  $k_1$ .

Theorem 5.1.2 of the upcoming chapter imposes the restrictions  $a \in L_{\infty,loc}([N, \infty))$  and  $b \in L_{\infty,loc}([N, \infty) \times [N, \infty))$ , with  $\alpha(R)$  and  $\beta(R)$  being the essential suprema for  $a$  and  $b$  on the restricted domains  $[N, R]$  and  $[N, R] \times [N, R]$  respectively. This being the case, we have  $A_i \leq \alpha(R)$  and  $B_{k,i} \leq \beta(R)$  for all values of  $i$  and  $k$  admissible in (4.16). Furthermore, from (4.6) we may deduce that each  $\tilde{B}_{j,i} \leq R$ . Finally, all mesh midpoints  $x_i$  must clearly satisfy  $x_i \geq N \geq 1 > h$ . Taken

together, these bounds lead, via a simple calculation, to

$$\frac{h}{\alpha(R) (\beta(R)R(R-N) + RN(N+1)/2)} \leq \frac{x_i}{A_i \left( \sum_{k=0}^{i-1} x_k B_{k,i} \Delta x_k + \sum_{j=1}^N j \tilde{B}_{j,i} \right)},$$

for  $i = 0, 1, \dots, I_h - 1$ . Hence, we have established a possible value for  $k_1$ , which allows (4.5) and (4.16) to be satisfied simultaneously as  $h \searrow 0$ .

### 4.3.2 Mass Conservation in the Numerical Solutions

In Lemma 3.5.2 of the previous chapter, the exact solution to our system of equations (3.1) and (3.2) was shown to conserve mass between the two regimes. We now show that this property is shared by our discrete approximating solutions.

**Lemma 4.3.3.** *The approximate solutions generated by (4.8) and (4.13) conserve mass.*

*Proof.* The mass associated with the approximate continuous regime solution,  $u_C^h(x, t)$ , is given by

$$\begin{aligned} \|u_C^h(\cdot, t)\|_{L^1_1(N, R)} &= \int_N^R \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) \chi_{\tau_n}(t) u_C^{n,i} x \, dx \\ &= \sum_{n=0}^{M-1} \chi_{\tau_n}(t) \sum_{i=0}^{I_h-1} u_C^{n,i} \int_N^R \chi_{\Lambda_i}(x) x \, dx \\ &= \sum_{n=0}^{M-1} \chi_{\tau_n}(t) \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n,i}, \end{aligned} \quad (4.18)$$

whilst the approximate solution  $u_D^h(t)$  has associated mass given by

$$\|u_D^h(t)\|_{X_D} = \sum_{i=1}^N i u_{D_i}^h(t) = \sum_{i=1}^N i \sum_{n=0}^{M-1} \chi_{\tau_n}(t) u_D^{n,i} = \sum_{n=0}^{M-1} \chi_{\tau_n}(t) \sum_{i=1}^N i u_D^{n,i}.$$

Summing these two expressions gives the total mass:

$$M^h(t) = \sum_{n=0}^{M-1} \chi_{\tau_n}(t) \left( \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n,i} + \sum_{i=1}^N i u_D^{n,i} \right). \quad (4.19)$$

First let us examine the mass accounted for by the continuous regime. From the

relation (4.8) we get

$$\begin{aligned}
\sum_{i=0}^{I_h-1} x_i u_C^{n+1,i} \Delta x_i &= \sum_{i=0}^{I_h-1} x_i \left( u_C^{n,i} + \frac{\Delta t}{x_i \Delta x_i} (F_{i+1/2}^n - F_{i-1/2}^n) - \frac{\Delta t}{x_i} S_i^n \right) \Delta x_i \\
&= \sum_{i=0}^{I_h-1} x_i u_C^{n,i} \Delta x_i + \Delta t \sum_{i=0}^{I_h-1} (F_{i+1/2}^n - F_{i-1/2}^n) - \Delta t \sum_{i=0}^{I_h-1} S_i^n \Delta x_i \\
&= \sum_{i=0}^{I_h-1} x_i u_C^{n,i} \Delta x_i - \Delta t \sum_{i=0}^{I_h-1} S_i^n \Delta x_i. \tag{4.20}
\end{aligned}$$

The middle summation term is lost in going to the final line as the sum is telescoping with zero end terms. Now we consider the discrete regime mass; the generating relation (4.13) gives us

$$\begin{aligned}
\sum_{i=1}^N i u_D^{n+1,i} &= \sum_{i=1}^N i \left( (1 - \Delta t a_i) u_D^{n,i} + \Delta t \sum_{j=i+1}^N a_j b_{i,j} u_D^{n,j} + \Delta t \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \Delta x_j \right) \\
&= \sum_{i=1}^N i u_D^{n,i} - \Delta t \sum_{i=1}^N i a_i u_D^{n,i} + \Delta t \sum_{i=1}^N i \sum_{j=i+1}^N a_j b_{i,j} u_D^{n,j} + \Delta t \sum_{i=1}^N i \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \Delta x_j \\
&= \sum_{i=1}^N i u_D^{n,i} - \Delta t \sum_{i=2}^N i a_i u_D^{n,i} + \Delta t \sum_{j=2}^N a_j u_D^{n,j} \left( \sum_{i=1}^{j-1} i b_{i,j} \right) \\
&\quad + \Delta t \sum_{j=0}^{I_h-1} \Delta x_j \left( A_j u_C^{n,j} \sum_{i=1}^N i \tilde{B}_{i,j} \right) \\
&= \sum_{i=1}^N i u_D^{n,i} + \Delta t \sum_{j=0}^{I_h-1} \Delta x_j S_j^n. \tag{4.21}
\end{aligned}$$

The middle two terms cancel due to the mass conservation condition (3.4). Combining equations (4.20) and (4.21) we obtain

$$\begin{aligned}
&\sum_{i=0}^{I_h-1} x_i u_C^{n+1,i} \Delta x_i + \sum_{i=1}^N i u_D^{n+1,i} \\
&= \sum_{i=0}^{I_h-1} x_i u_C^{n,i} \Delta x_i - \Delta t \sum_{i=0}^{I_h-1} S_i^n \Delta x_i + \sum_{i=1}^N i u_D^{n,i} + \Delta t \sum_{j=0}^{I_h-1} \Delta x_j S_j^n \\
&= \sum_{i=0}^{I_h-1} x_i u_C^{n,i} \Delta x_i + \sum_{i=1}^N i u_D^{n,i}.
\end{aligned}$$

From repeated application of this equality it is easily seen that the bracketed expression appearing in (4.19) is equal for all values of  $n$ , and hence the total mass  $M^h(t)$  remains constant.  $\square$

In this chapter we introduced a numerical scheme for the approximate solution of a truncated version of the system of equations from the previous chapter. Based around a finite volume discretisation of the continuous regime equation, (3.1), the associated numerical approximations were shown to retain non-negativity and conserve mass, provided the mesh satisfied certain constraints. In the following chapter we set out to establish, rigorously, the convergence of these solutions, as the mesh is refined.

# Chapter 5

## Numerical Approximation: Convergence of Numerical Solutions on the Truncated Domain

In the previous chapter we introduced a numerical scheme for the approximate solution of a truncated version of our equations (3.1) and (3.2). We proved that, provided certain criteria were met, these approximate solutions displayed the properties we would expect given the physical nature of the model. In this chapter we set out to prove that these approximate solutions converge, in some sense, to a limit as the parameter  $h$ , and by necessity  $\Delta t$ , go to zero and show that the limit itself is an ‘exact’ solution to our truncated model.

### 5.1 Continuous Fragmentation Regime: Convergence

Let us start with the continuous regime approximations  $\{u_C^h\}$ . In order to prove the (weak) convergence of this family, we employ a weak compactness argument, utilising the Dunford–Pettis theorem (Theorem 2.1.20), which provides necessary and sufficient conditions for weak compactness in an  $L_1$  space. We begin by proving the boundedness of the set  $\{u_C^h\}$ .

**Lemma 5.1.1.** *The family of approximations  $\{u_C^h\}$  is equibounded (uniformly bounded) in the space  $L_1((N, R) \times [0, T], x \, dx \, dt)$ .*

*Proof.* Recalling equation (4.18), we have for any  $t \in [0, T)$  that

$$\|u_C^h(\cdot, t)\|_{L_1^1(N, R)} = \sum_{n=0}^{M-1} \chi_{\tau_n}(t) \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n, i}.$$

From the analysis of the previous chapter, each of the values  $u_C^{n,i}$  is non-negative, and as such the values  $S_i^n$ , as defined in (4.7), are non-negative. Therefore, from the last line of equation (4.20) we deduce that

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n,i} \leq \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n-1,i} \quad \text{for } n = 1, \dots, M-1.$$

Repeated application of this inequality yields

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n,i} \leq \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{0,i} = \sum_{i=0}^{I_h-1} x_i \int_{\Lambda_i} c_0(x) dx \leq \sum_{i=0}^{I_h-1} \frac{x_i}{x_{i-1/2}} \int_{\Lambda_i} c_0(x) x dx. \quad (5.1)$$

The quantity  $\frac{x_i}{x_{i-1/2}}$  can be bounded as follows:

$$\frac{x_i}{x_{i-1/2}} = \frac{x_{i-1/2} + \frac{1}{2}\Delta x_i}{x_{i-1/2}} \leq 1 + \frac{h}{2N} \leq \frac{3}{2}. \quad (5.2)$$

We note this bound as it will appear regularly in subsequent calculations. Substituting this within (5.1) yields

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n,i} \leq \frac{3}{2} \|c_0\|_{L_1^+(N,R)},$$

for  $n = 0, \dots, M-1$ . Replacing this inequality in our calculation gives us the following, which holds for all  $t \in [0, T)$ :

$$\|u_C^h(\cdot, t)\|_{L_1^+(N,R)} \leq \sum_{n=0}^{M-1} \chi_{\tau_n}(t) \frac{3}{2} \|c_0\|_{L_1^+(N,R)} = \frac{3}{2} \|c_0\|_{L_1^+(N,R)}.$$

Integrating this inequality with respect to  $t$  from 0 to  $T$  we obtain the required equiboundedness of  $\{u_C^h\}$  in the space  $L_1((N, R) \times [0, T], x dx dt)$ .  $\square$

We now move on to prove the second of the two required conditions for the Dunford–Pettis theorem, namely equiintegrability.

**Theorem 5.1.2.** *Suppose that in addition to the restrictions of the previous chapter we have  $a \in L_{\infty,loc}([N, \infty))$  and  $b \in L_{\infty,loc}([N, \infty) \times [N, \infty))$ , and there exists a constant  $\theta > 0$  such that*

$$K(R)\Delta t \leq \theta < 1,$$

where  $K(R) = \alpha(R)\beta(R)R$ , with  $\alpha(R)$  and  $\beta(R)$  being the essential suprema for  $a$  and  $b$  on the restricted domains  $[N, R]$  and  $[N, R] \times [N, R]$ , respectively. Then the family  $\{u_C^h\}$  is equiintegrable in  $L_1((N, R) \times [0, T], x dx dt)$ .

*Proof.* Consider the constant sequence comprising solely of the initial data  $c_0 \in L_1((N, R), x dx)$ . Clearly this sequence is convergent, therefore  $\{c_0\}$  forms a weakly sequentially compact set in  $L_1((N, R), x dx)$ . Hence by the de la Vallee Poussin theorem (Theorem 2.1.18) there exists a non-negative, convex function  $\Phi \in C^\infty([0, \infty))$ , with  $\Phi(0) = 0$  and  $\Phi'(0) = 1$  such that  $\Phi'$  is concave and satisfies

$$\frac{\Phi(x)}{x} \rightarrow \infty \text{ as } x \rightarrow \infty \text{ and } \int_N^R \Phi(c_0)(x) x dx < \infty.$$

A standard inequality (2.3), for  $C^1$  convex functions gives us

$$(u_C^{n+1,i} - u_C^{n,i}) \Phi'(u_C^{n+1,i}) \geq \Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i}).$$

Multiplying this by  $x_i \Delta x_i$  and summing over all  $i$  gives

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) \leq \sum_{i=0}^{I_h-1} x_i \Delta x_i ((u_C^{n+1,i} - u_C^{n,i}) \Phi'(u_C^{n+1,i})).$$

Using equation (4.8) we can rewrite this as

$$\begin{aligned} & \sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) \\ & \leq \sum_{i=0}^{I_h-1} x_i \Delta x_i \left( \frac{\Delta t}{x_i \Delta x_i} (F_{i+1/2}^n - F_{i-1/2}^n) - \frac{\Delta t}{x_i} S_i^n \right) \Phi'(u_C^{n+1,i}). \end{aligned} \quad (5.3)$$

Recalling the definition of  $S_i^n$  from (4.7), we see that this is non-negative. Additionally, Lemma 2.1.19(ii) and Lemma 4.3.1 give  $\Phi'(u_C^{n+1,i}) \geq 0$ , hence we can drop the term involving  $S_i^n$  from (5.3) and the inequality will still remain valid, giving us

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) \leq \sum_{i=0}^{I_h-1} \Delta t (F_{i+1/2}^n - F_{i-1/2}^n) \Phi'(u_C^{n+1,i}).$$

With some easy modification, equation (4.15) becomes the inequality

$$F_{i+1/2}^n - F_{i-1/2}^n \leq x_i \Delta x_i \sum_{j=i+1}^{I_h-1} A_j B_{i,j} u_C^{n,j} \Delta x_j,$$

which, if placed in the previous inequality, results in

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) \leq \Delta t \sum_{i=0}^{I_h-1} \sum_{j=i+1}^{I_h-1} x_i A_j B_{i,j} u_C^{n,j} \Delta x_i \Delta x_j \Phi'(u_C^{n+1,i}).$$

Utilising Lemma 2.1.19(i) with  $x = u_C^{n,j}$  and  $y = u_C^{n+1,i}$  and noting that the constants  $\alpha(R)$  and  $\beta(R)$  bound the average values  $A_j$  and  $B_{i,j}$ , we get

$$\begin{aligned} \sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) &\leq \alpha\beta\Delta t \sum_{i=0}^{I_h-1} \sum_{j=i+1}^{I_h-1} x_i \Delta x_i \Delta x_j u_C^{n,j} \Phi'(u_C^{n+1,i}) \\ &\leq \alpha(R)\beta(R)\Delta t \left( \sum_{i=0}^{I_h-1} \left( x_i \Delta x_i \Phi(u_C^{n+1,i}) \sum_{j=i+1}^{I_h-1} \Delta x_j \right) \right. \\ &\quad \left. + \sum_{i=0}^{I_h-1} \left( x_i \Delta x_i \sum_{j=i+1}^{I_h-1} \Delta x_j \Phi(u_C^{n,j}) \right) \right). \end{aligned}$$

As  $j$  is restricted to be greater than  $i$  we have  $x_j > x_i$  for admissible  $j$  and  $i$ . This allows us to switch  $x_i$  for  $x_j$  in the second term and take this within the inner summation. Following this we expand the summation over  $j$  to give

$$\begin{aligned} \sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) &\leq \alpha(R)\beta(R)\Delta t \left( \sum_{i=0}^{I_h-1} \left( x_i \Delta x_i \Phi(u_C^{n+1,i}) \sum_{j=i+1}^{I_h-1} \Delta x_j \right) \right. \\ &\quad \left. + \sum_{i=0}^{I_h-1} \left( \Delta x_i \sum_{j=i+1}^{I_h-1} x_j \Delta x_j \Phi(u_C^{n,j}) \right) \right) \\ &\leq \underbrace{\alpha(R)\beta(R)R}_{=K(R)} \Delta t \left( \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n+1,i}) + \sum_{j=0}^{I_h-1} x_j \Delta x_j \Phi(u_C^{n,j}) \right). \end{aligned}$$

If we change the index variable from  $j$  to  $i$  and re-arrange then we obtain

$$(1 - K(R)\Delta t) \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n+1,i}) \leq (1 + K(R)\Delta t) \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n,i}).$$

Some further manipulations produce

$$(1 - K(R)\Delta t) \sum_{i=0}^{I_h-1} x_i \Delta x_i (\Phi(u_C^{n+1,i}) - \Phi(u_C^{n,i})) \leq 2K(R)\Delta t \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n,i}).$$

By the initial assumption of this theorem we have  $1 - K(R)\Delta t > 0$  allowing us to divide through to get

$$\sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n+1,i}) \leq \left( 1 + \frac{2K(R)\Delta t}{1 - K(R)\Delta t} \right) \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n,i}).$$

Repeated application of this inequality yields

$$\begin{aligned} \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n+1,i}) &\leq \left(1 + \frac{2K(R)\Delta t}{1 - K(R)\Delta t}\right)^{n+1} \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{0,i}) \\ &\leq \exp\left(\frac{2K(R)\Delta t(n+1)}{1 - K(R)\Delta t}\right) \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{0,i}). \end{aligned}$$

For values of  $t$  in the interval  $\tau_n = [t_n, t_{n+1})$  this gives us

$$\begin{aligned} \int_N^R \Phi(u_C^h(x, t)) x dx &= \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{n,i}) \\ &\leq \exp\left(\frac{2K(R)t}{1 - K(R)\Delta t}\right) \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi(u_C^{0,i}) \\ &= \exp\left(\frac{2K(R)t}{1 - K(R)\Delta t}\right) \sum_{i=0}^{I_h-1} x_i \Delta x_i \Phi\left(\frac{1}{\Delta x_i} \int_{\Lambda_i} c_0(x) dx\right). \end{aligned}$$

An application of Jensen's inequality [55, Theorem 2.2] allows us to switch the order of  $\Phi$  and integration to get

$$\begin{aligned} \int_N^R \Phi(u_C^h(x, t)) x dx &\leq \exp\left(\frac{2K(R)t}{1 - K(R)\Delta t}\right) \sum_{i=0}^{I_h-1} x_i \int_{\Lambda_i} \Phi(c_0(x)) dx \\ &\leq \frac{3}{2} \exp\left(\frac{2K(R)t}{1 - K(R)\Delta t}\right) \sum_{i=0}^{I_h-1} \int_{\Lambda_i} \Phi(c_0(x)) x dx. \end{aligned}$$

By our initial assumption that  $K(R)\Delta t \leq \theta < 1$ , we deduce that

$$\int_N^R \Phi(u_C^h(x, t)) x dx \leq \frac{3}{2} \exp\left(\frac{2K(R)t}{1 - \theta}\right) \int_N^R \Phi(c_0(x)) x dx,$$

which holds for all  $t \in [0, T)$ . Integrating the inequality with respect to  $t$  from 0 to  $T$  confirms the equiintegrability of the family  $\{u_C^h\}$  in the space  $L_1((N, R) \times [0, T), x dx dt)$ .  $\square$

By Theorem 2.1.20 (Dunford–Pettis theorem), the sequence  $\{u_C^h\}$  forms a weakly sequentially compact set which implies the existence of a subsequence  $\{u_C^{h_j}\}$  and a function  $u_C^R \in L_1((N, R) \times [0, T), x dx dt)$  such that  $u_C^{h_j} \rightharpoonup u_C^R$  in the space  $L_1((N, R) \times [0, T), x dx dt)$  as  $j \rightarrow \infty$  and  $h_j \rightarrow 0$ .

*Remark 5.1.3.* From now on this convergent subsequence will be considered implicitly, unless otherwise stated; as such we now use the notation  $\{u_C^h\}$  to denote such a convergent subsequence, the choice of which, we note, may not be unique.

## 5.2 Continuous Fragmentation Regime: Weak Solution

Having shown that our sequence of approximations converges (weakly) to a limit, we now aim to show that this limit provides a solution to our truncated equation (4.2). Precisely, we intend to show that the function  $u_C^R$  satisfies the following criterion.

**Definition 5.2.1.** The function  $u_C^R$  is a weak solution of equation (4.2), if it satisfies

$$\begin{aligned} & \int_0^T \int_N^R x u_C^R(x, t) \frac{\partial \varphi}{\partial t}(x, t) \, dx \, dt + \int_N^R x c_0(x) \varphi(x, 0) \, dx \\ &= \int_0^T \int_N^R \mathcal{F}^R(x u_C^R)(x, t) \frac{\partial \varphi}{\partial x}(x, t) \, dx \, dt + \int_0^T \int_N^R S(x u_C^R)(x, t) \varphi(x, t) \, dx \, dt, \end{aligned} \quad (5.4)$$

for all twice continuously differentiable functions  $\varphi$  with compact support in  $[N, R] \times [0, T]$ . This form was arrived at in the usual manner, recalling the zero boundary conditions established in Lemma 4.1.1.

**Definition 5.2.2.** In the analysis which follows we make use of the following three approximations to  $x$  over the domain  $[N, R]$ . First we have the left endpoint approximation, defined by

$$\xi^h : x \in [N, R] \rightarrow \xi^h(x) = \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) x_{i-1/2}.$$

Secondly we consider the midpoint approximation, defined by

$$X^h : x \in [N, R] \rightarrow X^h(x) = \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) x_i,$$

and finally we introduce the right endpoint approximation given by

$$\Xi^h : x \in [N, R] \rightarrow \Xi^h(x) = \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) x_{i+1/2}.$$

**Lemma 5.2.3.** *The three approximations  $\xi^h, X^h$  and  $\Xi^h$  introduced above, converge point-wise (uniformly) to  $x$  over the domain  $[N, R]$  as the mesh parameter  $h$  goes to 0.*

*Proof.* We consider only the case of  $\Xi^h$ , the proofs of the other two approximations being essentially the same. For any  $x \in [N, R]$  we have

$$|\Xi(x) - x| = \left| \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) x_{i+1/2} - x \right| = \sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) |x_{i+1/2} - x|.$$

Given such an  $x$ , it must lie in exactly one of the sub-intervals, say  $\Lambda_j$ , the length of which cannot exceed  $h$ ; hence

$$\sum_{i=0}^{I_h-1} \chi_{\Lambda_i}(x) |x_{i+1/2} - x| = |x_{j+1/2} - x| \leq |x_{j+1/2} - x_{j-1/2}| \leq h.$$

From this we may deduce that  $\Xi(x)$  converges point-wise (uniformly) to  $x$  over  $[N, R]$  as  $h \rightarrow 0$ . As mentioned previously, the same argument can be applied to  $\xi^h$  and  $X^h$ .  $\square$

We are now in a position to proceed with our proof that  $u_C^R$  is a weak solution to (4.2).

**Definition 5.2.4.** Let  $\varphi \in C^2([N, R] \times [0, T])$  be a compactly supported test function. For sufficiently small  $\Delta t$ , the support of  $\varphi$  with respect to  $t$  lies within  $[0, t_{M-1}]$ . We define  $\varphi_i^n$  as an approximation of  $\varphi$  on  $\Lambda_i \times \tau_n$  by

$$\varphi_i^n = \frac{1}{\Delta t} \int_{\tau_n} \varphi(x_{i-1/2}, t) dt,$$

with  $\varphi_i^{M-1} = \varphi_i^M = 0$  for admissible  $i$  and define  $\varphi_{I_h}^n = 0$  for all  $n$ .

Rearranging equation (4.8), multiplying by  $\varphi_i^n$  and summing over  $n = 0, \dots, M-1$  and  $i = 0, \dots, I_h - 1$ , gives us

$$\sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} (x_i \Delta x_i (u_C^{n+1,i} - u_C^{n,i}) \varphi_i^n - \Delta t (F_{i+1/2}^n - F_{i-1/2}^n) \varphi_i^n + \Delta t \Delta x_i S_i^n \varphi_i^n) = 0.$$

Rearrangement of the summations and utilising the bounded support of  $\varphi$  and the zero boundary flux gives us the following equality:

$$\begin{aligned} & \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n+1,i} (\varphi_i^{n+1} - \varphi_i^n) + \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{0,i} \varphi_i^0 \\ & - \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \Delta t F_{i+1/2}^n (\varphi_{i+1}^n - \varphi_i^n) - \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \Delta t \Delta x_i S_i^n \varphi_i^n = 0. \end{aligned} \quad (5.5)$$

The above equality can be seen as the discrete equivalent of the weak formulation (5.4). Our approach now involves taking the limit as  $h \rightarrow 0$  of (5.5) and showing that we do indeed obtain (5.4) with  $u_C^R$  as a weak solution. Observing the terms of (5.4) we see that the integrals are with respect to the measure  $dx dt$  whilst we have shown that convergence occurs in the space with weighted measure  $x dx dt$ . At this point we highlight the use of Theorem 2.1.10 to switch spaces but retain convergence.

*Remark 5.2.5.* We now make note of a property of the function  $\varphi$  and its derivatives, which we will make use of in our analysis. As  $\varphi$  has compact support and is identically zero outwith this support, its derivatives, both first and second, must also be zero outwith the support. Now within this compact support,  $\varphi$  and its derivatives are continuous and so must be bounded functions.

**Theorem 5.2.6.** *Let the assumptions already made regarding the kernels  $a$  and  $b$  and the mesh sizes  $h$  and  $\Delta t$  be satisfied; then the function  $u_C^R$  obtained as the limit of the sequence  $\{u_C^h\}$ , is a weak solution of our equation, satisfying (5.4).*

*Proof.* Looking initially at the first two terms of (5.5), we can express them as follows:

$$\begin{aligned}
& \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{n+1,i} (\varphi_i^{n+1} - \varphi_i^n) + \sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{0,i} \varphi_i^0 \\
&= \underbrace{\sum_{i=0}^{I_h-1} x_i \Delta x_i u_C^{M,i} (\varphi_i^M - \varphi_i^{M-1})}_{=0} \\
&+ \sum_{n=0}^{M-2} \sum_{i=0}^{I_h-1} \int_{\tau_{n+1}} \int_{\Lambda_i} X^h(x) u_C^h(x, t) \frac{\varphi(\xi^h(x), t) - \varphi(\xi^h(x), t - \Delta t)}{\Delta t} dx dt \\
&+ \sum_{i=0}^{I_h-1} \int_{\Lambda_i} X^h(x) u_C^h(x, 0) \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(\xi^h(x), t) dt dx \\
&= \int_0^T \int_N \chi_{[\Delta t, T]}(t) X^h(x) u_C^h(x, t) \frac{\varphi(\xi^h(x), t) - \varphi(\xi^h(x), t - \Delta t)}{\Delta t} dx dt \\
&+ \int_N X^h(x) u_C^h(x, 0) \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(\xi^h(x), t) dt dx.
\end{aligned}$$

Considering the double integral, assuming that  $\varphi \in C^2([N, R] \times [0, T])$ , Taylor expansions of the  $\varphi$  terms about the point  $(x, t)$  give us

$$\varphi(\xi^h(x), t) = \varphi(x, t) + (\xi^h(x) - x) \frac{\partial \varphi}{\partial x}(x, t) + O(h^2),$$

$$\varphi(\xi^h(x), t - \Delta t) = \varphi(x, t) + (\xi^h(x) - x) \frac{\partial \varphi}{\partial x}(x, t) + (t - \Delta t - t) \frac{\partial \varphi}{\partial t}(x, t) + O(h^2, h\Delta t, \Delta t^2).$$

Simple cancellations and recalling the condition (4.5) relating  $h$  and  $\Delta t$  give us

$$\frac{\varphi(\xi^h(x), t) - \varphi(\xi^h(x), t - \Delta t)}{\Delta t} = \frac{\Delta t \frac{\partial \varphi}{\partial t}(x, t) + O(\Delta t^2)}{\Delta t} \rightarrow \frac{\partial \varphi}{\partial t}(x, t), \quad (5.6)$$

as the mesh size goes to 0. Since the derivative  $\varphi_t$  is bounded, we can bound the left-hand side of (5.6) as  $h \rightarrow 0$ . From Lemma 5.2.3,  $\chi_{[\Delta t, T]}(t) X^h(x)$  can be seen

to converge pointwise to  $x$  on  $(0, T) \times (N, R)$  as  $h \rightarrow \infty$  and is clearly bounded by  $R$ . We have shown previously that  $u_C^h \rightharpoonup u_C^R$  in  $L_1((N, R) \times [0, T], x \, dx \, dt)$  and by Theorem 2.1.10 this is also the case in  $L_1((N, R) \times [0, T], dx \, dt)$  and so an application of Theorem 2.1.15 gives us

$$\begin{aligned} \int_0^T \int_N \chi_{[\Delta t, T]}(t) X^h(x) u_C^h(x, t) \frac{\varphi(\xi^h(x), t) - \varphi(\xi^h(x), t - \Delta t)}{\Delta t} \, dx \, dt \rightarrow \\ \int_0^T \int_N x u_C^R(x, t) \frac{\partial \varphi}{\partial t}(x, t) \, dx \, dt, \end{aligned} \quad (5.7)$$

as the mesh size parameter  $h$  goes to 0. Next, we consider the second term appearing above. Since  $\varphi$  is  $C^2([N, R] \times [0, T])$  with compact support, its derivatives are bounded, allowing us to deduce

$$\frac{1}{\Delta t} \int_0^{\Delta t} \varphi(\xi^h(x), t) \, dt \rightarrow \varphi(x, 0) \text{ as } h \searrow 0, \quad (5.8)$$

for all  $x \in [N, R]$ . Consider the following:

$$\begin{aligned} & \left| \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(\xi^h(x), t) \, dt - \varphi(x, 0) \right| = \left| \frac{1}{\Delta t} \int_0^{\Delta t} (\varphi(\xi^h(x), t) - \varphi(x, 0)) \, dt \right| \\ &= \left| \frac{1}{\Delta t} \int_0^{\Delta t} (\varphi(\xi^h(x), t) - \varphi(x, t) + \varphi(x, t) - \varphi(x, 0)) \, dt \right| \\ &\leq \frac{1}{\Delta t} \int_0^{\Delta t} |\varphi(\xi^h(x), t) - \varphi(x, t)| \, dt + \frac{1}{\Delta t} \int_0^{\Delta t} |\varphi(x, t) - \varphi(x, 0)| \, dt. \end{aligned} \quad (5.9)$$

Expressing  $\varphi(\xi^h(x), t)$  using a Taylor expansion about  $(x, t)$ , and recalling Remark 5.2.5 about the derivatives of  $\varphi$  we get

$$\varphi(\xi^h(x), t) = \varphi(x, t) + (\xi^h(x) - x) \frac{\partial \varphi}{\partial x}(x, t) + O(h^2).$$

Hence bounding the derivative  $\partial \varphi / \partial x$  and noting  $|\xi^h(x) - x| \leq h$ , gives us

$$|\varphi(\xi^h(x), t) - \varphi(x, t)| \leq C_1 h,$$

for some constant  $C_1$ . Similarly, expanding  $\varphi(x, t)$  about  $(x, 0)$  produces

$$\varphi(x, t) = \varphi(x, 0) + \underbrace{(t - 0)}_{\leq \Delta t} \frac{\partial \varphi}{\partial t}(x, 0) + O(h^2).$$

This leads to

$$|\varphi(x, t) - \varphi(x, 0)| \leq C_2 h,$$

for some other constant  $C_2$ . Returning to (5.9) we have

$$\left| \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(\xi^h(x), t) dt - \varphi(x, 0) \right| \leq (C_1 + C_2)h.$$

Hence (5.8) does indeed hold, furthermore the convergence is uniform with respect to  $x$ . From Lemma 5.2.3, we have the pointwise convergence of  $X^h(x)$  to  $x$  and Lemma 4.2.2 gives us the strong convergence in  $L_1(N, R)$  of  $u_C^h(x, 0)$  to the restriction of  $c_0$  to  $(N, R)$ . Therefore, another application of Theorem 2.1.15 yields

$$\int_N^R X^h(x) u_C^h(x, 0) \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(\xi^h(x), t) dt dx \rightarrow \int_N^R x c_0(x) \varphi(x, 0) dx. \quad (5.10)$$

Moving on to the third term of equation (5.5), for  $t \in \tau_n$  and  $x \in \Lambda_i$  we can write the numerical flux as an integral as follows:

$$\begin{aligned} F_{i+1/2}^n &= \sum_{j=i+1}^{I_h-1} \sum_{k=0}^i x_k A_j B_{k,j} u_C^{n,j} \Delta x_k \Delta x_j \\ &= \sum_{j=i+1}^{I_h-1} \sum_{k=0}^i \int_{\Lambda_j} \int_{\Lambda_k} X^h(w) a^h(v) b^h(w|v) u_C^h(v, t) dw dv \\ &= \int_{x_{i+1/2}}^R \int_N^{x_{i+1/2}} X^h(w) a^h(v) b^h(w|v) u_C^h(v, t) dw dv \\ &= \int_N^R \int_N^R \chi_{[\Xi^h(x), R]}(v) \chi_{[N, \Xi^h(x)]}(w) X^h(w) a^h(v) b^h(w|v) u_C^h(v, t) dw dv \\ &=: \mathcal{F}^h(u_C^h)(x, t). \end{aligned}$$

Then the third term of equation (5.5) is given by

$$\begin{aligned} &\sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \Delta t F_{i+1/2}^n (\varphi_{i+1}^n - \varphi_i^n) \\ &= \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} F_{i+1/2}^n \int_{\tau_n} \varphi(x_{i+1/2}, t) - \varphi(x_{i-1/2}, t) dt \\ &= \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \int_{\tau_n} \int_{\Lambda_i} F_{i+1/2}^n \frac{\partial \varphi}{\partial x}(x, t) dx dt \\ &= \int_0^T \int_N^R \mathcal{F}^h(u_C^h)(x, t) \frac{\partial \varphi}{\partial x}(x, t) dx dt. \end{aligned}$$

Expressed in full this gives us the following, after a switch in the order of integration:

$$\begin{aligned}
& \int_0^T \int_N \int_N \int_N (\chi_{[\Xi^h(x), R]}(v) \chi_{[N, \Xi^h(x)]}(w) X^h(w) \times \\
& \quad a^h(v) b^h(w|v) u_C^h(v, t)) \, dw \, dv \, \frac{\partial \varphi}{\partial x}(x, t) \, dx \, dt \\
&= \int_N \int_N \chi_{[N, \Xi^h(x)]}(w) X^h(w) \times \\
& \quad \left( \int_0^T \int_N \chi_{[\Xi^h(x), R]}(v) a^h(v) b^h(w|v) u_C^h(v, t) \frac{\partial \varphi}{\partial x}(x, t) \, dv \, dt \right) \, dw \, dx. \quad (5.11)
\end{aligned}$$

Due to the boundedness of the partial derivative  $\varphi_x$  and the  $L_{\infty, loc}$  property of the functions  $a$  and  $b$ , for almost all fixed  $(x, w) \in (N, R) \times (N, R)$ , the product  $\chi_{[\Xi^h(x), R]}(v) a^h(v) b^h(w|v) \frac{\partial \varphi}{\partial x}(x, t)$  is a bounded (uniformly w.r.t.  $h$ ) function of  $v$  and  $t$ . Also, thanks to Lemma 4.2.1 and Lemma 5.2.3 it converges pointwise almost everywhere to  $\chi_{[x, R]}(v) a(v) b(w|v) \frac{\partial \varphi}{\partial x}(x, t)$  as  $h \rightarrow 0$ . Since  $u_C^h \rightharpoonup u_C^R$  in  $L_1((N, R) \times (0, T), dx dt)$ , an application of Theorem 2.1.15 gives us

$$\begin{aligned}
& \int_0^T \int_N \chi_{[\Xi^h(x), R]}(v) a^h(v) b^h(w|v) u_C^h(v, t) \frac{\partial \varphi}{\partial x}(x, t) \, dv \, dt \\
& \quad \rightarrow \int_0^T \int_N \chi_{[x, R]}(v) a(v) b(w|v) u_C^R(v, t) \frac{\partial \varphi}{\partial x}(x, t) \, dv \, dt.
\end{aligned}$$

Using the local boundedness of  $a$  and  $b$ , along with the boundedness of the partial derivative  $\frac{\partial \varphi}{\partial x}$ , and the boundedness of the sequence  $\{u_C^h\}$  in  $L_1((N, R) \times (0, T), dx dt)$ , the left-hand side above can be bounded by a constant. It is easily seen that  $\chi_{[N, \Xi^h(x)]}(w) X^h(w)$  converges pointwise to  $\chi_{[N, x]}(w) w$  as  $h \rightarrow 0$  and can be bounded by  $R$  over our domain of interest. Therefore applying the Lebesgue dominated convergence theorem [55, Theorem 1.8], we get that (5.11) converges to

$$\begin{aligned}
& \int_N \int_N \chi_{[N, x]}(w) w \left( \int_0^T \int_N \chi_{[x, R]}(v) a(v) b(w|v) u_C^R(v, t) \frac{\partial \varphi}{\partial x}(x, t) \, dv \, dt \right) \, dw \, dx \\
&= \int_0^T \int_N \left( \int_x^R \int_N w a(v) b(w|v) u_C^R(v, t) \, dw \, dv \right) \frac{\partial \varphi}{\partial x}(x, t) \, dx \, dt \\
&= \int_0^T \int_N \mathcal{F}^R(x u_C^R)(x, t) \frac{\partial \varphi}{\partial x}(x, t) \, dx \, dt. \quad (5.12)
\end{aligned}$$

Therefore in the limit as  $h \rightarrow 0$ , the third term of (5.5) coincides with the third term of (5.4).

Now the fourth term from equation (5.5) is given fully by

$$\begin{aligned}
& \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} A_i \left( \sum_{j=1}^N j \tilde{B}_{j,i} \right) u_C^{n,i} \varphi_i^n \Delta x_i \Delta t \\
&= \sum_{n=0}^{M-1} \sum_{i=0}^{I_h-1} \int_{\tau_n} \int_{\Lambda_i} a^h(v) \left( \sum_{j=1}^N j b_j^h(v) \right) u_c^h(v, t) \varphi(\xi^h(v), t) dv dt \\
&= \int_0^T \int_N a^h(v) \left( \sum_{j=1}^N j b_j^h(v) \right) u_c^h(v, t) \varphi(\xi^h(v), t) dv dt.
\end{aligned}$$

The pointwise convergence of  $a^h$ ,  $b_j^h$  and  $\xi^h$  along with the continuity of  $\varphi$  means that

$$a^h(v) \left( \sum_{j=1}^N j b_j^h(v) \right) \varphi(\xi^h(v), t) \rightarrow a(v) \left( \sum_{j=1}^N j b_j(v) \right) \varphi(v, t),$$

for all  $t \in [0, T)$  and almost all  $v \in (R, N)$  as  $h \rightarrow 0$ . Since  $a$  and  $b_i$  are in  $L_{\infty,loc}([N, \infty))$  and  $\varphi$  is  $C^2$  on  $[N, R] \times [0, T)$  with compact support (hence is a bounded function), the expressions on either side belong to  $L_{\infty}((N, R) \times (0, T))$ , with the left-hand side being uniformly bounded w.r.t.  $h$ . Hence, with  $u_c^h \rightharpoonup u_C^R$  in  $L_1((N, R) \times (0, T), dv dt)$ , applying Theorem 2.1.15, yields

$$\begin{aligned}
& \int_0^T \int_N a^h(v) \left( \sum_{j=1}^N j b_j^h(v) \right) u_c^h(v, t) \varphi(\xi^h(v), t) dv dt \\
& \rightarrow \int_0^T \int_N a(v) \left( \sum_{j=1}^N j b_j(v) \right) u_c^R(v, t) \varphi(v, t) dv dt \\
&= \int_0^T \int_N S(vu_C^R)(v, t) \varphi(v, t) dv dt. \tag{5.13}
\end{aligned}$$

Taken together (5.7), (5.10), (5.12) and (5.13) show that  $u_C^R$  satisfies (5.5) for all compactly supported  $\varphi \in C^2([N, R] \times [0, T))$ , and hence  $u_C^R$  is a weak solution.  $\square$

### 5.3 Discrete Fragmentation Regime: Convergence

Now let us consider the discrete regime approximations. This is treated by a similar approach to the one we adopted for the continuous regime equation, but as a first step we establish a bound on the values  $u_D^{n,i}$ .

**Lemma 5.3.1.** *There exists a constant  $C$ , independent of  $h$  and  $R$ , such that for all values of  $n$  and  $i$  we have*

$$0 \leq u_D^{n,i} \leq C.$$

*Proof.* The non-negativity of  $u_D^{n,i}$  follows from Lemma 4.3.1. We shall therefore concentrate on the upper bound. From Lemma 4.3.3 we have, for all admissible  $n$ , that the following holds:

$$\begin{aligned}
\sum_{i=0}^{I_{h-1}} x_i \Delta x_i u_C^{n,i} + \sum_{i=1}^N i u_D^{n,i} &= \sum_{i=0}^{I_{h-1}} x_i \Delta x_i u_C^{0,i} + \sum_{i=1}^N i u_D^{0,i} \\
&= \sum_{i=0}^{I_{h-1}} x_i \int_{\Lambda_i} c_0(x) dx + \sum_{i=1}^N i d_{0i} \\
&\leq \frac{3}{2} \sum_{i=0}^{I_{h-1}} \int_{\Lambda_i} c_0(x) x dx + \sum_{i=1}^N i d_{0i} \\
&\leq \frac{3}{2} \int_N^\infty c_0(x) x dx + \sum_{i=1}^N i d_{0i} = C < \infty.
\end{aligned}$$

Therefore, for all  $n$  and  $i$  we have that

$$u_D^{n,i} \leq C,$$

where the constant  $C$  is independent of the mesh parameter  $h$  and the truncation parameter  $R$ .  $\square$

**Theorem 5.3.2.** *For each  $i = 1, \dots, N$ , the family  $\{u_{D_i}^h\}$  forms a sequentially weakly compact set in  $L_1(0, T)$ , hence must have a weakly convergent subsequence.*

*Proof.* The bound obtained in Lemma 5.3.1 allows us to easily establish equiboundedness and equiintegrability in  $L_1(0, T)$  for each of the families  $\{u_{D_i}^h\}$  as follows:

$$\|u_{D_i}^h(\cdot)\|_{L_1(0, T)} = \sum_{n=0}^{M-1} u_D^{n,i} \Delta t \leq \sum_{n=0}^{M-1} C \Delta t = CT. \quad (5.14)$$

Now let  $\Phi$  be any function of the nature described in Theorem 2.1.18. Since  $\Phi$  is increasing, the established bound for  $u_D^{n,i}$  allows us to deduce that

$$\int_0^T \Phi(u_{D_i}^h(t)) dt = \sum_{n=0}^{M-1} \Phi(u_D^{n,i}) \Delta t \leq \sum_{n=0}^{M-1} \Phi(C) \Delta t = \Phi(C)T. \quad (5.15)$$

Hence each of the families  $\{u_{D_i}^h\}$  are equiintegrable. By the Dunford–Pettis theorem (Theorem 2.1.20), the families form weakly sequentially compact sets in  $L_1(0, T)$ . As such, they all contain some weakly convergent subsequence.  $\square$

*Remark 5.3.3.* We note that what we seek is a collection of values  $\{h^j\}$ , such that all of the sequences  $\{u_{D_i}^{h^j}\}$ , for  $i = 1, \dots, N$ , converge weakly, as  $j \rightarrow \infty$  and  $h_j \rightarrow 0$ .

We achieve this by means of a diagonal argument, which we now outline. Knowing that the family  $\{u_{D_1}^h\}$  has a weakly convergent subsequence, let us denote the corresponding sequence of  $h$ -values by  $\{h^j\}_{j=1}^\infty$  and consider the family  $\{u_{D_2}^{h^j}\}_{j=1}^\infty$ . As this set satisfies the equiboundedness and equiintegrability conditions of the Dunford–Pettis theorem, it too must have a weakly convergent subsequence. Extracting this subsequence and denoting the corresponding  $h$ -values by  $\{h^{j_n}\}_{n=1}^\infty$ , we then have both  $\{u_{D_1}^{h^{j_n}}\}$  and  $\{u_{D_2}^{h^{j_n}}\}$  converging (weakly) as  $n \rightarrow \infty$  and  $j_n \rightarrow \infty$ . We can continue this process, working through each of the families  $\{u_{D_i}^h\}$ , until we have a set of common  $h$ -values,  $\{h'_j\}_{j=1}^\infty$ , for which all the subsequences  $\{u_{D_i}^{h'_j}\}_{j=1}^\infty$  are (weakly) convergent as  $j \rightarrow \infty$  and  $h'_j \rightarrow 0$ .

From now on these convergent subsequences are considered implicitly and we use  $\{u_{D_i}^h\}$  to denote said subsequences, unless otherwise stated. Let us denote the weak limit of  $\{u_{D_i}^h\}$  by  $u_{D_i}^R$  (note the upper case superscript notation for the limit).

## 5.4 Discrete Fragmentation Regime: Weak Solution

Having established the convergence of our sequence of approximations we now aim to determine whether the limit produced provides a solution to the equation (4.4) and if so in what sense. To this end, and mirroring the definition given for the continuous regime, we introduce the following definition of a solution of our discrete equation.

**Definition 5.4.1.** We say that the function  $u_{D_i}^R$  is a *weak* solution of equation (4.4) if it satisfies

$$\begin{aligned} & \int_0^T u_{D_i}^R(t) \frac{d\phi}{dt}(t) dt + d_{0_i} \phi(0) - \int_0^T a_i u_{D_i}^R(t) \phi(t) dt \\ & + \int_0^T \sum_{j=i+1}^N a_j b_{i,j} u_{D_j}^R(t) \phi(t) dt + \int_0^T \int_N^R a(y) b_i(y) u_C^R(y, t) \phi(t) dy dt = 0 \end{aligned} \quad (5.16)$$

for any  $C^2([0, T])$  function  $\phi$  with compact support.

**Theorem 5.4.2.** *The functions  $u_{D_i}^R$  obtained as weak limits of the sequences  $\{u_{D_i}^h\}$  are indeed weak solutions of (4.4), satisfying equation (5.16) for any compactly supported  $\phi \in C^2([0, T])$ .*

*Proof.* For such a function  $\phi$ , let us denote its approximation over  $\tau_n$  by  $\phi^n$ , which is defined as

$$\phi^n = \frac{1}{\Delta t} \int_{\tau_n} \phi(t) dt \text{ for } n = 0, \dots, M-1,$$

and  $\phi^M = 0$ . Multiplying (4.13) by  $\phi^n$  and summing over  $n$  from 0 to  $M-1$ , gives us the following equality:

$$\begin{aligned} & \sum_{n=0}^{M-1} (u_D^{n+1,i} - u_D^{n,i}) \phi^n = - \sum_{n=0}^{M-1} a_i u_D^{n,i} \phi^n \Delta t \\ & + \sum_{n=0}^{M-1} \sum_{j=i+1}^N a_j b_{i,j} u_D^{n,j} \phi^n \Delta t + \sum_{n=0}^{M-1} \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \phi^n \Delta x_j \Delta t. \end{aligned}$$

Since  $\phi$  is compactly supported, for sufficiently small  $\Delta t$  we have  $\phi^{M-1} = 0$ ; then, further manipulation of the first term yields

$$\begin{aligned} & \sum_{n=0}^{M-1} u_D^{n+1,i} (\phi^{n+1} - \phi^n) + u_D^{0,i} \phi^0 - \sum_{n=0}^{M-1} a_i u_D^{n,i} \phi^n \Delta t \\ & + \sum_{n=0}^{M-1} \sum_{j=i+1}^N a_j b_{i,j} u_D^{n,j} \phi^n \Delta t + \sum_{n=0}^{M-1} \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \phi^n \Delta x_j \Delta t = 0. \end{aligned} \quad (5.17)$$

Looking more closely at the first term above we can rewrite it as

$$\begin{aligned} \sum_{n=0}^{M-1} u_D^{n+1,i} (\phi^{n+1} - \phi^n) &= \underbrace{u_D^{M,i} (\phi^M - \phi^{M-1})}_{=0} + \sum_{n=0}^{M-2} \int_{\tau_{n+1}} u_{D_i}^h(t) \frac{\phi(t) - \phi(t - \Delta t)}{\Delta t} dt \\ &= \int_0^T \chi_{[\Delta t, T]}(t) u_{D_i}^h(t) \frac{\phi(t) - \phi(t - \Delta t)}{\Delta t} dt. \end{aligned}$$

A Taylor series expansion of  $\phi(t - \Delta t)$  about  $t$  gives

$$\phi(t - \Delta t) = \phi(t) - \Delta t \frac{d\phi}{dt}(t) + O(\Delta t^2).$$

Therefore we have

$$\frac{\phi(t) - \phi(t - \Delta t)}{\Delta t} = \frac{\Delta t \frac{d\phi}{dt}(t) + O(\Delta t^2)}{\Delta t} \rightarrow \frac{d\phi}{dt}(t),$$

as  $h$ , and by condition (4.5),  $\Delta t$  goes to 0. By an analogous argument to that used for  $\varphi$  and its derivatives,  $\phi$  and its derivative  $\phi_t$  must be bounded, therefore we can bound the left-hand side above. Also,  $\chi_{[\Delta t, T]}(t) \rightarrow 1$  on  $(0, T)$  as  $h$  and  $\Delta t \rightarrow 0$  and is clearly bounded. Then, as  $u_{D_i}^h \rightarrow u_{D_i}^R$  in  $L_1(0, T)$ , applying Theorem 2.1.15 gives us

$$\int_0^T \chi_{[\Delta t, T]}(t) u_{D_i}^h(t) \frac{\phi(t) - \phi(t - \Delta t)}{\Delta t} dt \rightarrow \int_0^T u_{D_i}^R(t) \frac{d\phi}{dt}(t) dt. \quad (5.18)$$

By definition,  $u_{D_i}^n = d_{0_i}$ , and since  $\phi$  is  $C^2$  with compact support, its derivative must be bounded, from which we deduce that

$$\phi^0 = \frac{1}{\Delta t} \int_0^{\Delta t} \phi(t) dt \rightarrow \phi(0),$$

as  $h$  goes to 0. Therefore

$$u_D^{n,i} \phi^0 \rightarrow d_{0_i} \phi(0) \text{ as } h \rightarrow 0. \quad (5.19)$$

By defining  $b_{i,i}$  to be  $-1$ , we can combine the third and fourth terms of (5.17), writing them as

$$\begin{aligned} \sum_{n=0}^{M-1} \sum_{j=i}^N a_j b_{i,j} u_D^{n,j} \phi^n \Delta t &= \sum_{n=0}^{M-1} \sum_{j=i}^N \int_{\tau_n} u_{D_j}^h(t) \phi(t) dt \\ &= \int_0^T \sum_{j=i}^N a_j b_{i,j} u_{D_j}^h(t) \phi(t) dt, \end{aligned}$$

and since  $u_{D_j}^h \rightharpoonup u_{D_j}^R$  in  $L_1(0, T)$ , for each  $j$ , we have

$$\begin{aligned} \int_0^T \sum_{j=i}^N a_j b_{i,j} u_{D_j}^h(t) \phi(t) dt &\rightarrow \int_0^T \sum_{j=i}^N a_j b_{i,j} u_{D_j}^R(t) \phi(t) dt \\ &= - \int_0^T a_i u_{D_i}^R(t) \phi(t) dt + \int_0^T \sum_{j=i+1}^N a_j b_{i,j} u_{D_j}^R(t) \phi(t) dt, \end{aligned} \quad (5.20)$$

giving us the third and fourth terms of our weak formulation (5.16). Rewriting the final term of our discrete relation, we get

$$\begin{aligned} \sum_{n=0}^{M-1} \sum_{j=0}^{I_h-1} A_j \tilde{B}_{i,j} u_C^{n,j} \phi^n \Delta x_j \Delta t &= \sum_{n=0}^{M-1} \sum_{j=0}^{I_h-1} \int_{\tau_n} \int_{\Lambda_j} a^h(y) b_i^h(y) \phi(t) u_C^h(y, t) dy dt \\ &= \int_0^T \int_N^R a^h(y) b_i^h(y) \phi(t) u_C^h(y, t) dy dt. \end{aligned}$$

We know from Lemma 4.2.1 that  $a^h(y)$  and  $b_i^h(y)$  converge pointwise to  $a(y)$  and  $b_i(y)$  respectively, and along with  $\phi$  are bounded (uniformly with respect to  $h$ ), a final application of Theorem 2.1.15 allows us to deduce that

$$\int_0^T \int_N^R a^h(y) b_i^h(y) \phi(t) u_C^h(y, t) dy dt \rightarrow \int_0^T \int_N^R a(y) b_i(y) u_C^R(y, t) \phi(t) dy dt, \quad (5.21)$$

as the mesh size parameter  $h \rightarrow 0$ . Taking the results (5.18), (5.19), (5.20) and (5.21), we see that by letting  $h \rightarrow 0$  in (5.17) we obtain the weak formulation (5.16), hence  $u_{D_i}^R$  is indeed a weak solution of (4.4).  $\square$

This chapter established the weak convergence of a subsequence of our approximate solutions as the mesh parameter was decreased to zero. The limits were shown to provide a set of weak solutions to the truncated versions of our equations of interest. However, there is some way to go, and a number of questions are yet unanswered. The convergence of subsequences rather than the full sequence raises the possibility of non-unique solutions, with each convergent subsequence possibly offering a different solution. Further, having obtained weak solutions we would like to establish whether these solutions may in fact display extra regularity, as we might expect from the results in Chapter 3. Finally, we should consider whether, by letting the truncation parameter  $R$  go to infinity, we obtain solutions to our full system. We shall look to address these questions in the next chapter.

## Chapter 6

# Convergence of Numerical Solutions as $R \rightarrow \infty$ and their relation to the Semigroup Solutions

In the previous two chapters, we approximated our system of equations on a truncated interval up to  $R$ . The numerically generated approximate solutions constructed on this interval were shown to converge to a weak solution on the restricted domain. We now consider what happens as we let the parameter  $R$  go to infinity. It is our aim to show that the truncated solutions  $u_C^R$  and  $u_D^R$  converge to solutions to the full equations (3.1) and (3.2) and hopefully determine how any solutions found relate to those obtained in Chapter 3 via the theory of semigroups.

### 6.1 Continuous Regime

Consider the following version of the continuous fragmentation equation (3.1):

$$\begin{aligned} \frac{\partial u_C^R(x, t)}{\partial t} &= -a_R(x)u_C^R(x, t) + \int_x^\infty a_R(y)b(x|y)u_C^R(y, t) dy, \quad x > N, \quad t > 0, \quad (6.1) \\ u_C^R(x, 0) &= c_0^R(x) := \chi_{(N, R)}(x)c_0(x), \end{aligned}$$

with the truncated fragmentation rate  $a_R(x)$  given by  $\chi_{(N, R)}(x)a(x)$ , where  $\chi_{(N, R)}$  is the characteristic function of the interval  $(N, R)$ . The above equation is equivalent to equation (4.1) from Chapter 4 and if we were to rewrite it in a conservative form, as we did in Chapter 4, then we would obtain an equation equivalent to the truncated equation (4.2).

From now on we shall assume that the parameter  $R$  is restricted to take only integer values as we let  $R \rightarrow \infty$ . As in Chapter 3 we shall reformulate our equation as an

abstract Cauchy problem in an  $L_1$  space. To this end let us introduce the following family of projection operators  $\{P_R\}$ , which act on  $X_C$  and are defined as follows. For  $f \in X_C$  we have

$$(P_R f)(x) = \chi_{(N,R)}(x)f(x) = \begin{cases} f(x) & \text{for } N < x < R, \\ 0 & \text{for } x \geq R. \end{cases}$$

Each projection operator maps the space  $X_C$  onto the subspace of  $X_C$  consisting of those elements which are zero over the interval  $[R, \infty)$ . This subspace, which we denote by  $X_C^R$ , is isometrically isomorphic to the space  $L_1((N, R), x dx)$  and for our purposes we may consider the spaces to be the same from now on, unless otherwise stated. Recalling the operators  $A_C$  and  $B_C$  from Chapter 3, we now define the linear operators  $A_C^R = A_C P_R = P_R A_C = P_R A_C P_R$  and  $B_C^R = P_R B_C P_R$  as truncated versions of  $A_C$  and  $B_C$  respectively, and additionally we define  $K_R = A_C^R + B_C^R$ . As a slight abuse of notation we simultaneously consider these operators acting on both of the spaces  $X_C$  and  $X_C^R$ .

We are assuming that the functions  $a$  and  $b$  retain the properties imposed in Theorem 5.1.2, that is  $a \in L_{\infty,loc}([N, \infty))$  and  $b \in L_{\infty,loc}([N, \infty) \times [N, \infty))$ . This leads to the following property for the operators  $A_C^R$  and  $B_C^R$ .

**Lemma 6.1.1.** *The operators  $A_C^R$  and  $B_C^R$  are bounded linear operators on the spaces  $X_C$  and  $X_C^R$ , with  $\|B_C^R f\| \leq \|A_C^R f\|$  for all  $f \in X_C$  or  $X_C^R$ , where the norm inequality holds for whichever space we are considering.*

*Proof.* We will first consider the operators on the space  $X_C^R$ . Let  $f \in X_C^R$ ; then we have

$$\begin{aligned} \|A_C^R f\|_{X_C^R} &= \int_N^R |a(x)\chi_{(N,R)}(x)f(x)| x dx \\ &= \int_N^R a(x) |f(x)| x dx \\ &\leq \alpha(R) \int_N^R |f(x)| x dx = \alpha(R) \|f\|_{X_C^R}. \end{aligned}$$

Therefore  $A_C^R$  is a bounded operator on the space  $X_C^R$ . The boundedness of  $B_C^R$  in  $X_C^R$  can be seen as follows. Let  $f \in X_C^R$ ; then

$$\begin{aligned} \|B_C^R f\|_{X_C^R} &= \int_N^R \left| \chi_{(N,R)}(x) \int_x^\infty a(y)b(x|y)\chi_{(N,R)}(y)f(y) dy \right| x dx \\ &\leq \int_N^R \left( \int_x^R a(y)b(x|y) |f(y)| dy \right) x dx \\ &= \int_N^R a(y) |f(y)| \left( \int_N^y x b(x|y) dx \right) dy \\ &\leq \int_N^R a(y) |f(y)| y dy \leq \|A_C^R f\|_{X_C^R} \leq \alpha(R) \|f\|_{X_C^R}. \end{aligned}$$

The change in order of integration can be justified by the non-negativity of the integrand along with Tonelli's theorem. The inequality in going from the third to the fourth line comes as a result of the mass conservation condition (3.3). The proof of the boundedness of  $A_C^R$  and  $B_C^R$  in  $X_C$  is essentially the same and we omit it for the sake of brevity.  $\square$

Equation (6.1) can then be recast as the following abstract Cauchy problem in either of the spaces  $X_C$  or  $X_C^R$ :

$$\frac{d}{dt}u_C^R(t) = (A_C^R + B_C^R)[u_C^R(t)], \quad t > 0; \quad u_C^R(0) = c_0^R = P_R c_0. \quad (6.2)$$

Here  $u_C^R : [0, \infty) \rightarrow X_C^R$  (or  $X_C$ ) denotes an  $X_C^R$  (or  $X_C$ )-valued function rather than the scalar-valued function of two variables from the previous section. However due to the relationship between the spaces  $L_1(I, L_1(\Omega, d\mu))$  and  $L_1(\Omega \times I, d\mu dt)$  detailed in Chapter 2 we may switch between the two, with each  $L_1$ -valued solution to (6.2) providing us with a scalar-valued solution to (6.1) and vice versa.

**Lemma 6.1.2.** *The operator  $(A_C^R + B_C^R)$  generates uniformly continuous semigroups of positive contractions on the spaces  $X_C^R$  and  $X_C$ .*

*Proof.* As a bounded linear operator on the space  $X_C^R$ , Theorem 2.4.7 tells us that  $A_C^R + B_C^R$  generates a uniformly continuous semigroup  $(T_R(t))_{t \geq 0}$  on  $X_C^R$ . The argument of Theorem 3.2.2 (Kato–Voigt perturbation theorem 2.5.22) is trivially adapted to the case  $(A_C^R + B_C^R, X_C^R)$  to give us that an ‘extension’ of  $(A_C^R + B_C^R, X_C^R)$  generates a substochastic semigroup. Now as  $A_C^R + B_C^R$  is defined and bounded on all of  $X_C^R$ , we must have that this extension is  $A_C^R + B_C^R$  itself and by Theorem 2.4.14, the substochastic semigroup generated must be  $(T_R(t))_{t \geq 0}$ . Hence  $(T_R(t))_{t \geq 0}$  is a uniformly continuous semigroup of positive contractions.

The same argument holds for  $(A_C^R + B_C^R, X_C)$  and we denote this semigroup generated on  $X_C$  by  $(S_R(t))_{t \geq 0}$ . Again this semigroup is uniformly continuous and consists of positive contractions.  $\square$

From the existence of the semigroup  $(T_R(t))_{t \geq 0}$  on  $X_C^R$ , Theorem 2.5.8 provides a unique strong solution to equation (6.2), given by  $u_C^R(t) = T_R(t)c_0^R$ . Additionally, by Theorem 2.5.10 this is also a unique mild solution, satisfying an equation of the form (2.17), in this case

$$u_C^R(t) = c_0^R + (A_C^R + B_C^R) \int_0^t u_C^R(s) ds = c_0^R + \int_0^t (A_C^R + B_C^R) u_C^R(s) ds, \quad (t \geq 0). \quad (6.3)$$

We are able to take the operator  $A_C^R + B_C^R$  inside the integral as a consequence of its boundedness by applying Lemma 2.3.4, hence our equation corresponds with the form of (2.14) from Definition 2.5.2.

**Theorem 6.1.3.** *The function  $u_C^R : [0, \infty) \rightarrow X_C^R$  provided by the semigroup  $(T_R(t))_{t \geq 0}$  is the unique weak solution to equation (6.2), satisfying Definition 2.5.4 over any time interval  $[0, T)$  where  $T < \infty$ .*

*Proof.* From the analysis above we have the semigroup  $(T_R(t))_{t \geq 0}$  providing a unique mild (strong) solution  $u_C^R : [0, \infty) \rightarrow X_C^R$  to equation (6.2). Theorem 2.5.6 tells us that if the right-hand side of (6.2) is integrable then, given either a weak or mild solution to our evolution equation, it can be modified on a set of measure zero to obtain a solution of the other form. Therefore in our case, if the conditions of Theorem 2.5.6 hold, the existence of a unique mild solution will provide a unique weak solution on each finite time interval  $[0, T)$ , with this solution being given by the semigroup  $(T_R(t))_{t \geq 0}$ .

Let  $0 < T < \infty$ ; utilising Theorem 2.2.10, we consider the following integral:

$$\begin{aligned}
& \int_0^T \|(A_C^R + B_C^R)u_C^R(s)\|_{X_C^R} ds \\
&= \int_0^T \int_N \left| -a(x)\chi_{(N,R)}(x)(u_C^R(s))(x) \right. \\
&\quad \left. + \chi_{(N,R)}(x) \int_x^\infty a(y)b(x|y)\chi_{(N,R)}(y)(u_C^R(s))(y) dy \right| x dx ds \\
&\leq \int_0^T \int_N a(x) |(u_C^R(s))(x)| x dx ds + \int_0^T \int_N \int_x^R a(y)b(x|y) |(u_C^R(s))(y)| dy x dx ds \\
&\leq \alpha(R) \int_0^T \int_N |(u_C^R(s))(x)| x dx ds + \alpha(R) \int_0^T \int_N \int_x^R b(x|y) |(u_C^R(s))(y)| dy x dx ds \\
&= \alpha(R) \int_0^T \int_N |(u_C^R(s))(x)| x dx ds + \alpha(R) \int_0^T \int_N |(u_C^R(s))(y)| \int_N^y b(x|y) x dx dy ds \\
&\leq 2\alpha(R) \int_0^T \int_N |(u_C^R(s))(x)| x dx ds \\
&= 2\alpha(R) \int_0^T \|T_R(s)c_0^R\|_{X_C^R} ds \leq 2\alpha(R)T \|c_0^R\|_{X_C^R} < \infty.
\end{aligned}$$

The bounding of the inner integral by  $y$  in the fifth line comes from the mass conservation condition (3.3), whilst the norm inequality utilised in the final line relies on the fact that the semigroup  $(T_R(t))_{t \geq 0}$  consists of contractions.

By Theorem 2.2.10 the right-hand side of equation (6.2) is integrable over the interval  $[0, T)$  and so by Theorem 2.5.6, any mild or weak solutions, as defined in Definitions 2.5.2 and 2.5.4, must agree (up to sets of measure zero). Therefore equation (6.2) has a unique weak solution given by  $u_C^R(t) = T_R(t)c_0^R$ , and this solution is in fact a strong solution.  $\square$

Let  $u_C^R(x, t)$  be a scalar representation of the semigroup solution  $(u_C^R(t))(x) = (T_R(t)c_0^R)(x)$ . Then applying Definition 2.5.4 to our example, noting Remark 2.5.5 and Appendix C, we get that equation (2.15) is equivalent to

$$\begin{aligned} & \int_0^T \int_N x u_C^R(x, t) \frac{\partial \varphi}{\partial t}(x, t) dx dt + \int_N x u_C^R(x, 0) \varphi(x, 0) dx \\ &= \int_0^T \int_N \mathcal{F}^R(x u_C^R(x, t))(x, t) \frac{\partial \varphi}{\partial x}(x, t) dx dt \\ & \quad + \int_0^T \int_N S(x u_C^R(x, t))(x, t) \varphi(x, t) dx dt, \end{aligned} \quad (6.4)$$

for all  $\varphi$  of the form  $\varphi(x, t) = \phi(x)\psi(t)$  where  $\phi \in C_c^\infty((N, R))$  and  $\psi \in C_c^\infty([0, T])$ , due to the weak-\* density of  $C_c^\infty((N, R))$  in  $L_\infty((N, R))$ , via Remark 2.5.5.

**Theorem 6.1.4.** *The weak solution obtained as the limit of the sequence of approximate solutions for the continuous regime in Theorems 5.1.2 and 5.2.6 is unique, continuously differentiable with respect to  $t$  on any interval  $[0, T)$  and satisfies equation (6.1) directly, except perhaps on a set of measure zero.*

*Proof.* It is easily seen that any scalar-valued function  $u_C^R(x, t)$  satisfying Definition 5.2.1 will immediately satisfy the equation (6.4) above. From any such scalar-valued function we may define a function  $u_C^R : [0, T) \rightarrow X_C^R$  via  $(u_C^R(t))(x) := u_C^R(x, t)$ , for almost all  $(x, t) \in (N, R) \times [0, T)$ . Since the scalar function satisfies equation (6.4), the  $X_C^R$ -valued function must provide a weak solution, as defined in Definition 2.5.4, to the abstract Cauchy problem (6.2). By Theorem 6.1.3, this weak solution must necessarily also be the unique (up to sets of measure zero) strong solution of (6.2). Hence for each scalar weak solution  $u_C^R(x, t)$  satisfying Definition 5.2.1 there is a unique corresponding  $X_C^R$ -valued strong solution  $u_C^R$  to the associated abstract Cauchy problem, whereby the original function  $u_C^R(x, t)$  is one scalar representation of the strong solution. Since the strong solution is unique, as are its scalar representations (up to measure zero), it follows that the weak solution must be unique, up to a set of measure zero. Further, as a representation of a strongly differentiable  $X_C^R$ -valued function, by Theorem 2.2.15,  $u_C^R(x, t)$  is continuously differentiable with respect to  $t$  (except perhaps on a set of zero measure) and by the same argument as applied in Theorem 3.2.7 directly satisfies equation (6.1) almost everywhere.  $\square$

This result greatly strengthens those of the previous section, where before we had only the existence of a (weakly) convergent subsequence and the possibility of the numerical scheme converging to multiple weak solutions. We now know that the limit solution must necessarily be unique, continuously differentiable with respect to  $t$  and a solution, in the classical sense, of the truncated fragmentation equation. Additionally it ties together the earlier analysis in this chapter with the semigroup theory of Chapter 3. We now aim to complete this tie-up by letting  $R \rightarrow \infty$  with

our truncated semigroup, hoping to obtain the semigroup  $(G_K(t))_{t \geq 0}$  obtained in Chapter 3. The approach adopted in this section follows a similar line of argument as that taken in [10, Section 8.3.2]. However, before we are able to establish the main result, we require some preliminary results and we begin with the following lemma.

**Lemma 6.1.5.** *For  $R \geq \tilde{R}$  and for  $t \geq 0$ , we have  $P_{\tilde{R}}T_R(t)P_{\tilde{R}} = T_{\tilde{R}}(t)$ .*

*Proof.* Firstly, for any  $f \in X_C$  and  $R > N$  we have

$$B_C P_R f = \int_x^\infty a(y)b(x|y)(P_R f)(y) dy = \int_x^R a(y)b(x|y)f(y) dy,$$

for  $N < x < R$  and  $B_C P_R f = 0$  for  $x \geq R$ , therefore  $B_C P_R f = P_R B_C P_R f$ . Whilst we have already noted that  $A_C P_R f = P_R A_C P_R f$ , as a result we have

$$K P_R = P_R K P_R = K_R. \quad (6.5)$$

It is easily seen from the definition of the projection operators that for  $R \geq \tilde{R}$  we get

$$P_{\tilde{R}} P_R = P_R P_{\tilde{R}} = P_{\tilde{R}}. \quad (6.6)$$

Together (6.5) and (6.6) give us

$$P_{\tilde{R}} K_R P_{\tilde{R}} = P_{\tilde{R}} (P_R K P_R) P_{\tilde{R}} = (P_{\tilde{R}} P_R) K (P_R P_{\tilde{R}}) = P_{\tilde{R}} K P_{\tilde{R}} = K_{\tilde{R}}. \quad (6.7)$$

We now generalise this relation using an inductive argument. Let us assume that  $P_{\tilde{R}}(K_R)^{n-1}P_{\tilde{R}} = (K_{\tilde{R}})^{n-1}$ , which in combination with (6.5) and (6.6) allows us to deduce that

$$\begin{aligned} P_{\tilde{R}}(K_R)^n P_{\tilde{R}} &= P_{\tilde{R}}(K_R)^{n-1} K_R P_{\tilde{R}} \\ &= P_{\tilde{R}}(K_R)^{n-1} (P_R K P_R) P_{\tilde{R}} && \text{by (6.5)} \\ &= P_{\tilde{R}}(K_R)^{n-1} P_R K (P_{\tilde{R}} P_R) && \text{by (6.6)} \\ &= P_{\tilde{R}}(K_R)^{n-1} P_R (P_{\tilde{R}} K P_{\tilde{R}}) P_R && \text{by (6.5)} \\ &= P_{\tilde{R}}(K_R)^{n-1} P_{\tilde{R}} (K P_{\tilde{R}}) && \text{by (6.6)} \\ &= P_{\tilde{R}}(K_R)^{n-1} P_{\tilde{R}} K_{\tilde{R}} && \text{by (6.5)} \\ &= (K_{\tilde{R}})^{n-1} K_{\tilde{R}} && \text{by assumption} \\ &= (K_{\tilde{R}})^n. \end{aligned}$$

Hence by induction  $P_{\tilde{R}}(K_R)^n P_{\tilde{R}} = (K_{\tilde{R}})^n$  for positive all integers  $n$ , when  $R \geq \tilde{R}$ . Additionally we note that the relation also holds for  $n = 0$ , where  $(K_R)^0$  is the appropriate identity operator for the space we are considering. Since the operator  $K_{\tilde{R}}$  is a bounded linear operator, the semigroup  $T_{\tilde{R}}(t)$  that it generates is given by the exponential formula (2.10). Utilising the relation just established, we obtain the desired result as follows:

$$T_{\tilde{R}}(t) = \sum_{n=0}^{\infty} \frac{t^n (K_{\tilde{R}})^n}{n!} = \sum_{n=0}^{\infty} \frac{t^n P_{\tilde{R}}(K_R)^n P_{\tilde{R}}}{n!} = P_{\tilde{R}} \left( \sum_{n=0}^{\infty} \frac{t^n (K_R)^n}{n!} \right) P_{\tilde{R}} = P_{\tilde{R}} T_R(t) P_{\tilde{R}}.$$

□

The semigroup  $(T_R(t))_{t \geq 0}$  can be extended to form a family of uniformly continuous operators on the space  $X_C$  by

$$\bar{T}_R(t) = P_R T_R(t) P_R. \quad (6.8)$$

However,  $(\bar{T}_R(t))_{t \geq 0}$  does not form a semigroup on  $X_C$ , as setting  $t = 0$  does not produce the identity operator on  $X_C$ . But as noted previously, the truncated operator  $K_R$  does generate a uniformly continuous semigroup  $(S_R(t))_{t \geq 0}$  on  $X_C$ . Given  $f \in X_C$ , the operator  $K_R$  acts as the zero operator on  $f$  over  $[R, \infty)$ , hence for the part of  $f$  supported in  $[R, \infty)$ ,  $(S_R(t))_{t \geq 0}$  acts as the identity operator. We can decompose  $f \in X_C$  as  $f = P_R f + (I_C - P_R)f$ , where  $I_C$  denotes the identity operator on  $X_C$ . We then obtain the following relationship between the families  $(S_R(t))_{t \geq 0}$  and  $(\bar{T}_R(t))_{t \geq 0}$ :

$$\begin{aligned} S_R(t)f &= \sum_{n=0}^{\infty} \frac{t^n (K_R)^n}{n!} P_R f + \sum_{n=0}^{\infty} \frac{t^n (K_R)^n}{n!} (I_C - P_R)f \\ &= P_R \sum_{n=0}^{\infty} \frac{t^n (K_R)^n}{n!} P_R f + (I_C - P_R)f \\ &= P_R T_R(t) P_R f + (I_C - P_R)f \\ &= \bar{T}_R(t)f + (I_C - P_R)f. \end{aligned} \quad (6.9)$$

For elements of  $X_C$  supported in  $(N, R)$ ,  $I_C - P_R$  acts as the zero operator, giving rise to the relation

$$S_R(t)P_R f = P_R T_R(t)P_R(P_R f) + (I_C - P_R)P_R f = P_R T_R(t)P_R f = \bar{T}_R(t)f. \quad (6.10)$$

The following lemma establishes a feature of the family  $(\bar{T}_R(t))_{t \geq 0}$  which will enable us to prove a number of significant properties of both  $(\bar{T}_R(t))_{t \geq 0}$  and  $(S_R(t))_{t \geq 0}$ , via the relations (6.9) and (6.10).

**Lemma 6.1.6.** *The family of operators  $(\bar{T}_R(t))_{t \geq 0}$  is increasing with  $R$ . That is, for  $f \in X_{C+}$  and fixed  $t \geq 0$  we have*

$$\bar{T}_R(t)f \geq \bar{T}_{\tilde{R}}(t)f, \quad \text{when } R \geq \tilde{R}.$$

*Proof.* Let  $f \in X_C$ , with  $f \geq 0$  and for  $R > N$  define

$$f_R(t) = P_R T_R(t) P_R f = \bar{T}_R(t)f \geq 0.$$

It is then easily seen from the monotonic nature of the projection operators that

$(P_{R+1} - P_R)f_{R+1}(t) \geq 0$ . Further, we may deduce that

$$\begin{aligned} \frac{d}{dt}f_{R+1}(t) &= \frac{d}{dt}(P_{R+1}T_{R+1}(t)P_{R+1}f) \\ &= P_{R+1}\frac{d}{dt}T_{R+1}(t)(P_{R+1}f) \\ &= P_{R+1}K_{R+1}T_{R+1}(t)P_{R+1}f \\ &= K_{R+1}P_{R+1}T_{R+1}(t)P_{R+1}f \\ &= K_{R+1}f_{R+1}(t), \end{aligned}$$

where the boundedness of  $P_{R+1}$  allowed us to switch its order with the derivative in going to the second line. We have made use of a standard property of semigroups (Theorem 2.4.11) in going to the third line, and finally (6.5) and the idempotence of the projection operators have been used to derive the fourth line. Utilising this, we obtain

$$\begin{aligned} \frac{d}{dt}P_Rf_{R+1}(t) &= P_R\frac{d}{dt}f_{R+1}(t) \\ &= P_RK_{R+1}f_{R+1}(t) \\ &= P_RK_{R+1}P_{R+1}f_{R+1}(t) \\ &= P_RK_{R+1}(P_R + P_{R+1} - P_R)f_{R+1}(t) \\ &= P_RK_{R+1}P_Rf_{R+1}(t) + P_RK_{R+1}(P_{R+1} - P_R)f_{R+1}(t). \end{aligned} \quad (6.11)$$

Since  $K_{R+1} = A_C^{R+1} + B_C^{R+1}$  and

$$\begin{aligned} P_RA_C^{R+1}P_{R+1} &= P_R(A_CP_{R+1})P_{R+1} = (P_RA_C)P_{R+1} \\ &= (P_RA_CP_R)P_{R+1} = P_RA_CP_{R+1}P_R = P_RA_C^{R+1}P_R, \end{aligned}$$

the second term on the right of (6.11) becomes

$$\begin{aligned} &P_RK_{R+1}(P_{R+1} - P_R)f_{R+1}(t) \\ &= P_RA_C^{R+1}(P_{R+1} - P_R)f_{R+1}(t) + P_RB_C^{R+1}(P_{R+1} - P_R)f_{R+1}(t) \\ &= P_RB_C^{R+1}(P_{R+1} - P_R)f_{R+1}(t). \end{aligned}$$

Then noting that  $P_RK_{R+1}P_R = K_R = K_RP_R$ , equation (6.11) becomes

$$\frac{d}{dt}P_Rf_{R+1}(t) = K_RP_Rf_{R+1}(t) + P_RB_C^{R+1}(P_{R+1} - P_R)f_{R+1}(t),$$

with  $P_Rf_{R+1}(0) = P_RP_{R+1}T_{R+1}(0)P_{R+1}f = P_Rf$ . Applying the Duhamel formula, in this case produces

$$\begin{aligned} P_Rf_{R+1}(t) &= T_R(t)P_Rf + \int_0^t T_R(s-t)P_RB_C^{R+1}(P_{R+1} - P_R)f_{R+1}(s) ds \\ &\geq T_R(t)P_Rf, \end{aligned}$$

which gives us the following inequality:

$$P_R f_{R+1}(t) = P_R P_R f_{R+1}(t) \geq P_R T_R(t) P_R f = \bar{T}_R(t) f.$$

Combined with our earlier statement that  $(P_{R+1} - P_R) f_{R+1}(t) \geq 0$  we arrive at

$$\bar{T}_{R+1}(t) f = f_{R+1}(t) = P_{R+1} f_{R+1}(t) \geq P_R f_{R+1}(t) \geq \bar{T}_R(t) f.$$

Hence the sequence  $(\bar{T}_R(t) f)_{R \in \mathbb{N} | R > N}$  is non-decreasing.  $\square$

At this point we take a brief diversion in order to establish a property of our truncated solutions, which we shall rely on for the analysis of the discrete component of our system, in the following section.

**Lemma 6.1.7.** *The strong solution  $S_R(t)c_0^R$ , of the truncated abstract Cauchy problem (6.2), in  $X_C$ , remains within  $D(K)$  for all  $t \geq 0$ .*

*Proof.* For all  $t \geq 0$ , we have

$$\begin{aligned} S_R(t)c_0^R &= S_R(t)P_R c_0 && \text{by the definition of } c_0^R \\ &= \bar{T}_R(t)c_0 && \text{by (6.10)} \\ &= P_R T_R(t)P_R c_0 && \text{by (6.8)} \\ &= P_R \underbrace{P_R T_R(t)P_R c_0}_{=S_R(t)c_0^R} && \text{by the idempotence of } P_R \\ &= P_R S_R(t)c_0^R. \end{aligned}$$

Therefore, we have the following relation:

$$K S_R(t)c_0^R = K P_R S_R(t)c_0^R = K_R S_R(t)c_0^R,$$

from the definition of  $K_R$  in (6.5). Since  $K_R$  is the generator of the semigroup  $(S_R(t))_{t \geq 0}$  in  $X_C$ , by Theorem 2.4.11, we have  $K_R S_R(t)c_0^R \in X_C$  and hence  $K S_R(t)c_0^R \in X_C$  for all  $t \geq 0$ . As such we may deduce that  $S_R(t)c_0^R \in D(K)$  for all  $t \geq 0$ .  $\square$

Returning to the matter at hand, we are now in a position to establish the convergence of both  $(\bar{T}_R(t))_{t \geq 0}$  and  $(S_R(t))_{t \geq 0}$  as we let  $R \rightarrow \infty$ .

**Theorem 6.1.8.** *There exists a strongly continuous semigroup  $(G(t))_{t \geq 0}$  of positive contractions on  $X_C$ , such that for  $f \in X_C$  and  $t \geq 0$ ,*

$$G(t)f = \lim_{R \rightarrow \infty} S_R(t)f = \lim_{R \rightarrow \infty} \bar{T}_R(t)f. \quad (6.12)$$

*Additionally, the convergence in both limits is uniform with respect to  $t$ , on bounded intervals. Further, when  $f_0 \in X_C^R$ , we have*

$$G(t)f_0 = P_R T_R(t)P_R f_0,$$

*for any  $R \geq \tilde{R}$ .*

*Proof.* Due to the substochastic nature of the semigroups  $(T_R(t))_{t \geq 0}$ , we have the bound

$$\|\bar{T}_R(t)f\|_{X_C} = \|T_R(t)f\|_{X_C^R} \leq \|P_R f\|_{X_C^R} \leq \|f\|_{X_C}.$$

As a non-decreasing, norm bounded sequence in the positive cone of the  $KB$ -space (Definition 2.1.7)  $X_C$ , the sequence  $(\bar{T}_R(t)f)_{R \in \mathbb{N}|R > N}$  must converge in  $X_C$  for each fixed  $t \geq 0$ . Hence, provided that  $f \geq 0$  we may define

$$G(t)f = \lim_{R \rightarrow \infty} \bar{T}_R(t)f, \quad t \geq 0. \quad (6.13)$$

Since any element of  $X_C$ , may be expressed as the difference of two elements of  $X_{C+}$ , this definition can be extended by linearity to all of  $X_C$ . Considering the additional term from equation (6.9), for fixed  $f \in X_C$  we have

$$(I_C - P_R)f = \begin{cases} f(x) & \text{for } x \geq R, \\ 0 & \text{for } N < x < R, \end{cases}$$

from which it is straightforward to see that  $|((I_C - P_R)f)(x)|$  converges point-wise to 0 as  $R \rightarrow \infty$  and is bounded above by  $|f(x)|$ . Applying Lebesgue's dominated convergence theorem gives us

$$\int_N^\infty |((I_C - P_R)f)(x)| x dx \rightarrow 0, \quad \text{as } R \rightarrow \infty.$$

That is,  $(I_C - P_R)f$  converges to zero in  $X_C$  as  $R$  goes to infinity. Taking the limit as  $R \rightarrow \infty$  of both sides of equation (6.9) yields

$$G(t)f = \lim_{R \rightarrow \infty} S_R(t)f, \quad t \geq 0, \quad (6.14)$$

for any  $f \in X_C$ . Therefore  $(G(t))_{t \geq 0}$  is obtained as the strong limit, in  $X_C$ , of uniformly continuous semigroups of positive contractions. By the continuity of the norm and the closed nature of the positive cone  $X_{C+}$ , the family of operators  $(G(t))_{t \geq 0}$  can be seen to consist of positive contractions. We now aim to show that  $(G(t))_{t \geq 0}$  forms a  $C_0$ -semigroup. Conditions (i) and (ii) of Definition 2.4.1 are easily established. Let,  $f \in X_C$ ; then

$$G(0)f = \lim_{R \rightarrow \infty} S_R(0)f = \lim_{R \rightarrow \infty} I_C f = f,$$

hence  $G(0)$  acts as the identity operator on  $X_C$ . Now for any fixed  $s, t \geq 0$ , we get

$$\begin{aligned} & \|S_R(t)S_R(s)f - G(t)G(s)f\|_{X_C} \\ &= \|S_R(t)S_R(s)f - S_R(t)G(s)f + S_R(t)G(s)f - G(t)G(s)f\|_{X_C} \\ &\leq \|S_R(t)S_R(s)f - S_R(t)G(s)f\|_{X_C} + \|S_R(t)G(s)f - G(t)G(s)f\|_{X_C} \\ &\leq \|S_R(t)\| \|S_R(s)f - G(s)f\|_{X_C} + \|S_R(t)(G(s)f) - G(t)(G(s)f)\|_{X_C} \\ &\leq \|S_R(s)f - G(s)f\|_{X_C} + \|S_R(t)(G(s)f) - G(t)(G(s)f)\|_{X_C}. \end{aligned}$$

The final step is justified as the semigroup  $(S_R(t))_{t \geq 0}$  consists of contractions. Letting  $R \rightarrow \infty$  above, recalling (6.14), we obtain

$$\lim_{R \rightarrow \infty} (S_R(t)S_R(s)f) = G(t)G(s)f,$$

and therefore

$$G(t+s)f = \lim_{R \rightarrow \infty} S_R(t+s)f = \lim_{R \rightarrow \infty} (S_R(t)S_R(s)f) = G(t)G(s)f.$$

It remains to establish condition (iii) of Definition 2.4.1. First let us assume that  $f \in X_{C+}$ , then set  $g = P_R f$ , further, let us take  $m \in \mathbb{N}$  such that  $m > R$ ; then we have

$$\begin{aligned} \|G(t)g - g\|_{X_C} &= \|G(t)g - \bar{T}_m(t)g + \bar{T}_m(t)g - g\|_{X_C} \\ &\leq \|G(t)g - \bar{T}_m(t)g\|_{X_C} + \|\bar{T}_m(t)g - g\|_{X_C} \\ &= \|G(t)g\|_{X_C} - \|\bar{T}_m(t)g\|_{X_C} + \|\bar{T}_m(t)g - g\|_{X_C} \\ &\leq \|g\|_{X_C} - \|S_m(t)g\|_{X_C} + \|\bar{T}_m(t)g - g\|_{X_C} \\ &\leq \|g - S_m(t)g\|_{X_C} + \|\bar{T}_m(t)g - g\|_{X_C}. \end{aligned}$$

The equality of the second and third lines above can be justified by the increasing nature of  $(\bar{T}_R(t))_{t \geq 0}$ , and the non-negativity of  $g$ . We then utilise the fact that  $(G(t))_{t \geq 0}$  consists of contractions as well as (6.10) to obtain the fourth line. Finally an application of the reverse triangle inequality yields the final line. As both  $(\bar{T}_m(t))_{t \geq 0}$  and  $(S_m(t))_{t \geq 0}$  are  $C_0$ -semigroups and satisfy condition (iii) of Definition 2.4.1 themselves, this quantity converges to zero as  $t \rightarrow 0^+$ . Now for general  $f \in X_C$  we set

$$g = P_R f = P_R f_+ - P_R f_- = g_+ - g_-, \quad \text{where } g_+ = P_R f_+ \text{ and } g_- = P_R f_-.$$

This leads to the following bounding estimate:

$$\begin{aligned} \|G(t)g - g\|_{X_C} &= \|(G(t)g_+ - g_+) - (G(t)g_- - g_-)\|_{X_C} \\ &\leq \|G(t)g_+ - g_+\|_{X_C} + \|G(t)g_- - g_-\|_{X_C}. \end{aligned}$$

By the same argument as we applied above for non-negative functions, this quantity must converge to zero as  $t \rightarrow 0^+$ . Now given any  $f \in X_C$ , clearly  $P_R f$  converges pointwise to  $f$  on  $(N, \infty)$  as  $R \rightarrow \infty$ , and  $P_R f$  is dominated by the integrable  $|f|$ , hence by Lebesgue's dominated convergence theorem

$$\|P_R f - f\|_{X_C} = \int_N^\infty |P_R f(x) - f(x)| x dx \rightarrow 0 \text{ as } R \rightarrow \infty.$$

Now given such an  $f$  and  $\epsilon > 0$ , let us take  $R \in \mathbb{N}$  such that  $\|P_R f - f\|_{X_C} < \epsilon/4$ , for then we have

$$\begin{aligned} \|G(t)f - f\|_{X_C} &= \|G(t)f - G(t)P_R f + G(t)P_R f - P_R f + P_R f - f\|_{X_C} \\ &\leq \|G(t)f - G(t)P_R f\|_{X_C} + \|G(t)P_R f - P_R f\|_{X_C} + \|P_R f - f\|_{X_C} \\ &\leq (\|G(t)\| + 1) \|P_R f - f\|_{X_C} + \|G(t)P_R f - P_R f\|_{X_C} \\ &\leq \epsilon/2 + \|G(t)P_R f - P_R f\|_{X_C}, \end{aligned}$$

where the final line was obtained by recalling that  $(G(t))_{t \geq 0}$  consists of contractions, and the assumption  $\|P_R f - f\|_{X_C} < \epsilon/4$ . By the previous result, the second term  $\|G(t)P_R f - P_R f\|_{X_C}$  can be made less than  $\epsilon/2$  by taking  $t$  to be sufficiently small. Then, for such  $t$ ,  $\|G(t)f - f\|_{X_C} < \epsilon$ , thus establishing condition (iii) of Definition 2.4.1.

Now let us suppose that for some  $f \in X_C$  the convergence of  $\bar{T}_R(t)f$  to  $G(t)f$  is not uniform with respect to  $t$  in some compact interval  $[\alpha, \beta]$ . Then there exists an  $\epsilon_0 > 0$  such that for any  $M \in \mathbb{N}$ , we can find  $m > M$  and  $t \in [\alpha, \beta]$  where

$$\|G(t)f - \bar{T}_m(t)f\|_{X_C} \geq \epsilon_0.$$

Incrementing  $M$  we form a sequence of  $m$ 's (increasing) and  $t$ 's, such that the above inequality holds for corresponding pairs  $(m, t)$ . The Bolzano-Weierstrass theorem allows us to extract subsequences  $\{m_n\}$  and  $\{t_n\}$ , such that  $m_n \rightarrow \infty$  (monotonically) and  $t_n \rightarrow \bar{t}$  as  $n \rightarrow \infty$ , for some  $\bar{t} \in [\alpha, \beta]$ .

Now let us assume that  $f \in X_{C+}$ ; then the non-decreasing nature of  $(\bar{T}_R(t))_{t \geq 0}$  established in Lemma 6.1.6 along with the previous inequality allow us to deduce the following relation:

$$\begin{aligned} \|G(t_n)f\|_{X_C} - \|\bar{T}_{m_n}(t_n)f\|_{X_C} &= \|G(t_n)f - \bar{T}_{m_n}(t_n)f\|_{X_C} \geq \epsilon_0 \\ \Rightarrow \|\bar{T}_{m_n}(t_n)f\|_{X_C} &\leq \|G(t_n)f\|_{X_C} - \epsilon_0, \end{aligned}$$

which holds for all values of  $n$ . However, for  $k < n$  we have  $0 \leq \bar{T}_{m_k}(t_n)f \leq \bar{T}_{m_n}(t_n)f$ , and therefore

$$\|\bar{T}_{m_k}(t_n)f\|_{X_C} \leq \|\bar{T}_{m_n}(t_n)f\|_{X_C},$$

which combined with the previous inequality yields

$$\|\bar{T}_{m_k}(t_n)f\|_{X_C} \leq \|G(t_n)f\|_{X_C} - \epsilon_0.$$

Letting,  $n \rightarrow \infty$ , we obtain

$$\|\bar{T}_{m_k}(\bar{t})f\|_{X_C} \leq \|G(\bar{t})f\|_{X_C} - \epsilon_0,$$

which holds for all values of  $k \in \mathbb{N}$ . An application of the reverse triangle inequality then provides us with

$$\|G(\bar{t})f - \bar{T}_{m_k}(\bar{t})f\|_{X_C} \geq \|G(\bar{t})f\|_{X_C} - \|\bar{T}_{m_k}(\bar{t})f\|_{X_C} \geq \epsilon_0.$$

This contradicts the convergence established previously in (6.13), and hence our assertion that convergence was not uniform must have been false. Now given a general  $f \in X_C$  we decompose it as  $f = f_+ - f_-$ . Then, for  $t$  restricted to some compact interval we can write

$$\begin{aligned} \|G(t)f - \bar{T}_R(t)f\|_{X_C} &= \|(G(t)f_+ - \bar{T}_R(t)f_+) - (G(t)f_- - \bar{T}_R(t)f_-)\|_{X_C} \\ &\leq \|G(t)f_+ - \bar{T}_R(t)f_+\|_{X_C} + \|G(t)f_- - \bar{T}_R(t)f_-\|_{X_C}. \end{aligned}$$

Now given  $\epsilon > 0$ , by our previous result on the uniform convergence for non-negative functions, there exist  $R_1$  and  $R_2$  such that for all  $t$  in our compact interval

$$\|G(t)f_+ - \bar{T}_R(t)f_+\|_{X_C} < \frac{\epsilon}{2}, \quad \text{for all } R > R_1,$$

and likewise with  $\|G(t)f_- - \bar{T}_R(t)f_-\|_{X_C}$  for  $R > R_2$ . Setting  $R_{max} = \max(R_1, R_2)$ , we get

$$\|G(t)f - \bar{T}_R(t)f\|_{X_C} < \frac{\epsilon}{2} + \frac{\epsilon}{2}, \quad \text{for } R > R_{max},$$

for all  $t$  in our compact interval. Hence as stated, convergence is uniform on compact intervals. To obtain the equivalent result for  $(S_R(t))_{t \geq 0}$ , it is enough to note that the discrepancy between  $(S_R(t))_{t \geq 0}$  and  $(\bar{T}_R(t))_{t \geq 0}$  as given in (6.9), is independent of  $t$ .

To prove the final result of this theorem we first consider  $T_R(t)P_{\tilde{R}}$  in the case that  $R \geq \tilde{R}$ . As the semigroup  $(T_R(t))_{t \geq 0}$  is uniformly continuous, it is given by the series (2.11), hence

$$T_R(t)P_{\tilde{R}} = \sum_{n=0}^{\infty} \frac{t^n (K_R)^n}{n!} P_{\tilde{R}}. \quad (6.15)$$

For the first term when  $n = 0$ , we have

$$(K_R)^0 P_{\tilde{R}} = I_R P_{\tilde{R}} = I_{\tilde{R}} = (K_{\tilde{R}})^0,$$

and with the  $n = 1$  term, we get

$$(K_R)^1 P_{\tilde{R}} = (K P_R) P_{\tilde{R}} = K P_{\tilde{R}} = (K_{\tilde{R}})^1,$$

from (6.5) and (6.6). Now let us suppose that for a general  $k \in \mathbb{N}$ , the following holds:

$$(K_R)^k P_{\tilde{R}} = (K_{\tilde{R}})^k;$$

then we may further deduce that

$$\begin{aligned}
(K_R)^{k+1}P_{\tilde{R}} &= K_R(K_R)^kP_{\tilde{R}} \\
&= K_R(K_{\tilde{R}})^k && \text{by assumption} \\
&= (KP_R)K_{\tilde{R}}(K_{\tilde{R}})^{k-1} && \text{by (6.5)} \\
&= (KP_R)(P_{\tilde{R}}KP_{\tilde{R}})(K_{\tilde{R}})^{k-1} && \text{by (6.5)} \\
&= (KP_{\tilde{R}})(KP_{\tilde{R}})(K_{\tilde{R}})^{k-1} && \text{by (6.6)} \\
&= K_{\tilde{R}}K_{\tilde{R}}(K_{\tilde{R}})^{k-1} && \text{by (6.5)} \\
&= (K_{\tilde{R}})^{k+1}.
\end{aligned}$$

Therefore by induction, the relation  $(K_R)^n P_{\tilde{R}} = (K_{\tilde{R}})^n$  holds for  $n = 0, 1, 2, \dots$ , and as such equation (6.15) becomes

$$T_R(t)P_{\tilde{R}} = \sum_{n=0}^{\infty} \frac{t^n (K_R)^n}{n!} P_{\tilde{R}} = \sum_{n=0}^{\infty} \frac{t^n (K_{\tilde{R}})^n}{n!} = T_{\tilde{R}}(t). \quad (6.16)$$

Having established this we are able to proceed to proving the final result of this theorem. Let us suppose that  $f_0 \in X_C^{\tilde{R}}$ , so we may write as  $f_0 = P_{\tilde{R}}f_0$ . Then for any  $R \geq \tilde{R}$  we have

$$\begin{aligned}
\bar{T}_R(t)f_0 &= P_R T_R(t) P_R f_0 && \text{by (6.8)} \\
&= T_R(t)f_0 && \text{by Lemma 6.1.5} \\
&= T_R(t)P_{\tilde{R}}f_0 \\
&= T_{\tilde{R}}(t)f_0 && \text{by (6.16)}.
\end{aligned}$$

Since this is independent of  $R$  provided  $R \geq \tilde{R}$ , taking the limit of the left-hand side as  $R \rightarrow \infty$  and utilising (6.12) gives us

$$G(t)f_0 = \lim_{R' \rightarrow \infty} \bar{T}_{R'}(t)f_0 = P_R T_R(t) P_R f_0,$$

for any  $R \geq \tilde{R}$ , as required.  $\square$

Having established the existence of a limit semigroup  $(G(t))_{t \geq 0}$  it remains to show that this semigroup coincides with the continuous regime semigroup  $(G_K(t))_{t \geq 0}$ , obtained in Chapter 3. As a first step towards this we demonstrate the minimality of  $(G(t))_{t \geq 0}$  in the following lemma.

**Lemma 6.1.9.** *Let  $u(x, t)$  be a non-negative-valued function, integrable on  $(N, R) \times [0, T)$  with respect to the measure  $x dx dt$  for any  $R > N$  and  $T > 0$ , such that  $u(x, t)$  satisfies the following integrated version of equation (3.1):*

$$u(x, t) = c_0(x) + \int_0^t (-a(x)u(x, s) + (\mathcal{B}u)(x, s)) ds, \quad (6.17)$$

for almost all  $x > N$  and  $t > 0$ , where  $\mathcal{B}u$  is the integral expression defined in (3.5) in Chapter 3, and where the initial mass distribution satisfies  $c_0 \in X_C$ . Then for all  $t \geq 0$  and almost all  $x$ , we have

$$u(x, t) \geq (G(t)c_0)(x). \quad (6.18)$$

*Proof.* From the assumption of the integrability and non-negativity of  $u$  and the  $L_{\infty,loc}([N, \infty))$  nature of  $a$ , Fubini's theorem gives us

$$\int_N^R \left( \int_0^t a(x)u(x, s) ds \right) x dx = \int_0^t \left( \int_N^R a(x)u(x, s)x dx \right) ds < \infty,$$

and

$$\int_N^R \left( \int_0^t (\mathcal{B}u)(x, s) ds \right) x dx = \int_0^t \left( \int_N^R (\mathcal{B}u)(x, s)x dx \right) ds < \infty, \quad (6.19)$$

for  $N < R < \infty$  and  $0 < t \leq T$ , therefore  $-au + \mathcal{B}u \in L_1((N, R) \times [0, T], x dx dt)$ . Now let us define the truncated function  $u_R(x, t) := \chi_{(N, R)}(x)u(x, t)$ , for  $R > N$ , which then satisfies the equation

$$\begin{aligned} u_R(x, t) &= \chi_{(N, R)}(x)c_0(x) + \chi_{(N, R)}(x) \left( \int_0^t (-a(x)u(x, s) + (\mathcal{B}u)(x, s)) ds \right) \\ &= \chi_{(N, R)}(x)c_0(x) + \int_0^t (-a(x)u_R(x, s) + (\mathcal{B}u_R)(x, s)) ds + \int_0^t f_R(x, s) ds, \end{aligned} \quad (6.20)$$

where, for  $s \geq 0$ , the function  $f_R(x, s)$  is given by

$$f_R(x, s) = \int_R^\infty a(y)b(x|y)u(y, s) dy \geq 0,$$

for  $N < x < R$  and  $f_R(x, s) = 0$  for  $x \geq R$ . By the non-negativity of  $u$  and (6.19) we have

$$\begin{aligned} \int_0^T \left( \int_N^\infty |f_R(x, s)| x dx \right) ds &= \int_0^T \left( \int_N^R \left( \int_R^\infty a(y)b(x|y)u(y, s) dy \right) x dx \right) ds \\ &\leq \int_0^T \left( \int_N^R \left( \int_x^\infty a(y)b(x|y)u(y, s) dy \right) x dx \right) ds = \int_0^T \left( \int_N^R (\mathcal{B}u)(x, s)x dx \right) ds < \infty. \end{aligned}$$

Therefore  $f_R \in L_1((N, \infty) \times [0, T], x dx dt)$  for each  $R > N$ . Now by Theorem 2.2.14, as  $u_R(x, t)$  is integrable, we can form an integrable function  $\bar{u}_R : [0, T] \rightarrow X_C$  defined for almost all  $t \in [0, T)$  by  $\bar{u}_R(t) := u_R(\cdot, t)$ , and likewise we can form  $\bar{f}_R : [0, T] \rightarrow X_C$  by  $\bar{f}_R(t) := f_R(\cdot, t)$ . Now let  $t$  and  $t + \tau$  lie within

$[0, T]$ ; then, utilising (6.20), we get

$$\begin{aligned} \|\bar{u}_R(t + \tau) - \bar{u}_R(t)\|_{X_C} &\leq \int_N^\infty \left( \int_t^{t+\tau} |-a(x)u_R(x, s) + (\mathcal{B}u_R)(x, s)| \, ds \right) x \, dx \\ &\quad + \int_N^\infty \left( \int_t^{t+\tau} f_R(x, s) \, ds \right) x \, dx \\ &= \int_N^R \left( \int_0^T \chi_{(t, t+\tau)}(s) |-a(x)u_R(x, s) + (\mathcal{B}u_R)(x, s)| \, ds \right) x \, dx \\ &\quad + \int_N^R \left( \int_0^T \chi_{(t, t+\tau)}(s) f_R(x, s) \, ds \right) x \, dx. \end{aligned}$$

Recalling that  $-au + \mathcal{B}u \in L_1((N, R) \times [0, T], x \, dx \, dt)$  and  $f_R \in L_1((N, \infty) \times [0, T], x \, dx \, dt)$  whence the integrands are bounded by integrable functions, and recognising that they converge pointwise to zero as  $\tau \rightarrow 0$ , the function  $\bar{u}_R : [0, T] \rightarrow X_C$  is strongly continuous in  $X_C$ .

Rewriting equation (6.20) whilst noting Remark 2.5.15, we see that  $\bar{u}_R : [0, T] \rightarrow X_C$  satisfies the following equation in  $X_C$ :

$$\bar{u}_R(t) = P_R c_0 + \int_0^t (A_C^R + B_C^R) \bar{u}_R(s) \, ds + \int_0^t \bar{f}_R(s) \, ds, \quad \text{for } 0 \leq t < T.$$

Therefore,  $\bar{u}_R : [0, T] \rightarrow X_C$  is a mild solution of the inhomogeneous abstract Cauchy problem

$$\frac{d}{dt} \bar{u}_R(t) = (A_C^R + B_C^R) [\bar{u}_R(t)] + \bar{f}_R(t), \quad t > 0; \quad \bar{u}_R(0) = P_R c_0.$$

As such,  $\bar{u}_R(t)$  is given by an application of (2.20). Hence we have

$$\bar{u}_R(t) = S_R(t) P_R c_0 + \int_0^t S_R(t-s) \bar{f}_R(s) \, ds, \quad (6.21)$$

where  $(S_R(t))_{t \geq 0}$  is the uniformly continuous, substochastic semigroup generated on  $X_C$  by  $A_C^R + B_C^R$ , from Lemma 6.1.2. Now as  $\bar{f}_R$  is non-negative and  $(S_R(t))_{t \geq 0}$  is substochastic, the integral term appearing on the right-hand side of equation (6.21) is also non-negative. Therefore  $\bar{u}_R(t) \geq S_R(t) P_R c_0$ , that is  $u_R(x, t) \geq (S_R(t) P_R c_0)(x)$ . Now  $u_R$  converges to  $u$  as  $R \rightarrow \infty$  and from (6.10) we get  $S_R(t) P_R c_0 = \bar{T}_R(t) c_0$ , which converges to  $G(t) c_0$  as  $R \rightarrow \infty$  as shown in Theorem 6.1.8. Putting these together we get that  $u(x, t) \geq (G(t) c_0)(x)$  as required.  $\square$

We are now in a position to show that the limit semigroup  $(G(t))_{t \geq 0}$  obtained in Theorem 6.1.8 coincides with the substochastic semigroup  $(G_K(t))_{t \geq 0}$  generated on  $X_C$  by  $K$ , as obtained in Chapter 3. In doing so we complete the link between the truncated equation (6.5) and its numerical solutions from Chapters 4 and 5, and the full equation (3.1) and its analytic solution from Chapter 3.

**Theorem 6.1.10.** *Under the assumptions so far imposed, the semigroups  $(G(t))_{t \geq 0}$  and  $(G_K(t))_{t \geq 0}$  agree on  $X_C$ , that is*

$$G(t)c_0 = G_K(t)c_0, \quad t \geq 0, \quad c_0 \in X_C.$$

*Proof.* First of all let us define  $X_0$  as the following subspace of  $X_C$ :

$$X_0 = \bigcup_{R > N} X_C^R.$$

This subspace forms a core, as defined in Definition 2.3.13, for the multiplication operator  $(A_C, D(A_C))$ , which we now demonstrate. Let  $f \in D(A_C)$ , and define the family  $\{f_R\}_{R > N}$  by  $f_R = P_R f$ . As each  $f_R \in X_C^R$ , we have  $\{f_R\} \subseteq X_0$ . Then we get

$$\begin{aligned} \|f_R - f\|_{A_C} &= \|f_R - f\|_{X_C} + \|A_C f_R - A_C f\|_{X_C} \\ &= \int_N^\infty |\chi_{(N,R)}(x)f(x) - f(x)| x dx + \int_N^\infty |\chi_{(N,R)}(x)a(x)f(x) - a(x)f(x)| x dx \\ &= \int_N^\infty \chi_{[R,\infty)}(x) |f(x)| x dx + \int_N^\infty \chi_{[R,\infty)}(x) |a(x)f(x)| x dx. \end{aligned}$$

The two integrands above are dominated by  $|f(x)|$  and  $|a(x)f(x)|$  respectively, both of which are integrable. The integrands also converge pointwise to zero as  $R \rightarrow \infty$ . Applying the Lebesgue dominated convergence theorem we get that  $\|f_R - f\|_{A_C} \rightarrow 0$  as  $R \rightarrow \infty$ . As such the subspace  $X_0$  is dense in  $D(A)$  for the graph norm  $\|\cdot\|_{A_C}$  and with that,  $X_0$  is a core for  $A_C$ .

Additionally, the subspace  $X_0$  is a subset of the domain of the generator of the semigroup  $(G(t))_{t \geq 0}$ . Firstly let  $(H, D(H))$  denote the generator of  $(G(t))_{t \geq 0}$ . Now suppose that  $f \in X_0$ , then we have  $f \in X_C^R$  for some  $R > N$  and we get

$$\begin{aligned} G(t)f &= P_R T_R(t) P_R f && \text{by Theorem 6.1.8} \\ &= \bar{T}_R(t) f && \text{by (6.8)} \\ &= S_R(t) f && \text{by (6.10)}. \end{aligned}$$

Hence, for this  $f \in X_0$  and  $t > 0$  we have

$$\frac{1}{t} (G(t)f - f) = \frac{1}{t} (S_R(t)f - f).$$

Recall that  $(S_R(t))_{t \geq 0}$  is generated on  $X_C$  by the bounded operator  $A_C^R + B_C^R$ . Therefore as we let  $t \searrow 0$  in the above equation we get

$$\lim_{t \rightarrow 0^+} \frac{1}{t} (G(t)f - f) = \lim_{t \rightarrow 0^+} \frac{1}{t} (S_R(t)f - f) = (A_C^R + B_C^R)f \in X_C.$$

Since the left-hand limit exists as an element in  $X_C$  we must have that  $f \in D(H)$ , and so  $X_0$  is a subset of  $D(H)$ . Furthermore, for such  $f$ , the generator  $H$  is given by

$$Hf = \lim_{t \rightarrow 0^+} \frac{1}{t} (G(t)f - f) = (A_C^R + B_C^R)f = (A_C + B_C)f,$$

since  $(A_C^R + B_C^R)$  and  $(A_C + B_C)$  agree on  $X_C^R$ . Therefore,  $(G(t))_{t \geq 0}$  is generated by an extension of  $(A_C + B_C, X_0)$  and as  $X_0$  is a core for  $A_C$  an application of Theorem 2.5.28 gives us

$$G(t)c_0 \geq G_K(t)c_0, \quad t \geq 0, \quad c_0 \in X_{C+}. \quad (6.22)$$

Now let us suppose that  $c_0 \in D(A_C)_+ \subseteq D(K)$ . Integrating equation (3.16) with respect to  $t$  we see that  $u_C(x, t) = [G_K(t)c_0](x)$  satisfies equation (6.17) of Lemma 6.1.9, thus

$$[G_K(t)c_0](x) \geq [G(t)c_0](x).$$

Putting this together with the inequality (6.22) we have

$$G(t)c_0 = G_K(t)c_0,$$

for  $c_0 \in D(A_C)_+$ . Since any element of  $D(A)$  can be expressed as the difference of two elements of  $D(A_C)_+$ , we may extend this equality to all of  $D(A_C)$ . Further still, using the density of  $D(A_C)$  we can extend it to all of  $X_C$  as required.  $\square$

Having shown convergence for the continuous regime as the truncation parameter  $R \rightarrow \infty$ , in the following section we establish similar results for the discrete regime equations.

## 6.2 Discrete Regime

Recalling the truncated discrete regime equation (4.4) from Chapter 4, we have for  $i = 1, \dots, N$ :

$$\begin{aligned} \frac{du_{D_i}^R(t)}{dt} &= -a_i u_{D_i}^R(t) + \sum_{j=i+1}^N a_j b_{i,j} u_D^R(t)_j + \int_N^\infty a_R(y) b_i(y) u_C^R(y, t) dy, \quad t > 0, \\ u_D^R(0) &= d_0. \end{aligned} \quad (6.23)$$

These equations are recast as the following inhomogeneous abstract Cauchy problem on the space  $X_D$  introduced in Chapter 3:

$$\frac{d}{dt} u_D^R(t) = (A_D + B_D)[u_D^R(t)] + C_R[u_C^R(t)], \quad t > 0; \quad u_D^R(0) = d_0, \quad (6.24)$$

where  $A_D$  and  $B_D$  are as defined in Chapter 3,  $u_C^R$  is the truncated semigroup solution of (6.2) and where  $C_R: D(C_R) \subseteq X_C \rightarrow X_D$  is given by

$$(C_R f)_i = \int_N^\infty a_R(y) b_i(y) f(y) dy, \quad D(C_R) = \{f \in X_C : C_R f \in X_D\} = X_C,$$

for  $i = 1, \dots, N$ . The fact that  $D(C_R) = X_C$  is a consequence of the construction of  $a_R$  in (6.1) and the  $L_{\infty,loc}$  boundedness of  $a$  along with the bound (4.6). Recall that since the space  $X_D$  is finite-dimensional, the operators  $A_D$  and  $B_D$  are bounded and therefore by Theorem 2.4.7 they must generate a uniformly continuous semigroup  $(T(t))_{t \geq 0}$  on  $X_D$ . We then consider the term  $C_R[u_C^R(t)]$  as a perturbation and (6.24) as an inhomogeneous abstract Cauchy problem of the form (2.18). The following lemma establishes the differentiability of this perturbation term, a property that we will require in showing the existence of solutions of equation (6.24), along with determining their nature.

**Lemma 6.2.1.** *The term  $C_R[u_C^R(t)]$  from (6.24) is strongly differentiable (in the space  $X_D$ ) with respect to  $t$ , at almost all points of  $[0, T]$ . Furthermore its derivative is given by  $C_R[\frac{d}{dt}u_C^R(t)]$ .*

*Proof.* Recalling the  $L_{\infty,loc}$  boundedness of  $a$  and the bound  $b_i(y) \leq y$  for each  $i \in \{1, 2, \dots, N\}$ , from (4.6), we have that

$$\begin{aligned} & \left| \frac{(C_R[u_C^R(t+h)])_i - (C_R[u_C^R(t)])_i}{h} - \left( C_R \left[ \frac{d}{dt} u_C^R(t) \right] \right)_i \right| \\ &= \left| \int_N a_R(y) b_i(y) \left( \frac{(u_C^R(t+h))(y) - (u_C^R(t))(y)}{h} - \left[ \frac{d}{dt} u_C^R(t) \right](y) \right) dy \right| \\ &\leq \alpha(R) \int_N \left| \frac{(u_C^R(t+h))(y) - (u_C^R(t))(y)}{h} - \left[ \frac{d}{dt} u_C^R(t) \right](y) \right| y dy \\ &= \alpha(R) \left\| \frac{u_C^R(t+h) - u_C^R(t)}{h} - \frac{d}{dt} u_C^R(t) \right\|_{X_C}, \end{aligned}$$

where  $\alpha(R)$  is the essential supremum of  $a$  over  $[N, R]$ . From the differentiability of  $u_C^R$ , by letting  $h \rightarrow 0$  on both sides of the above calculation, we may deduce that  $C_R[u_C^R(t)]$  is differentiable (in the space  $X_D$ ) at almost all points of  $[0, T]$ , with derivative  $C_R[\frac{d}{dt}u_C^R(t)]$ .  $\square$

Having shown the differentiability of the perturbation term  $C_R[u_C^R(t)]$ , we now look at its derivative more closely, showing that it is integrable, belonging to the space  $L_1((0, T), X_D)$  and in doing so establish the existence of a unique strong solution to equation (6.24).

**Theorem 6.2.2.** *The derivative of  $C_R[u_C^R(t)]$  belongs to the space  $L_1((0, T), X_D)$ . As such equation (6.24) has a unique strong solution, which is given by (2.20) with  $\varphi(t) = C_R[u_C^R(t)]$ .*

*Proof.* If we take the  $X_D$ -norm of the derivative  $\frac{d}{dt}C_R[u_C^R(t)]$  established in the previous lemma and integrate from 0 to  $T$ , then we obtain

$$\begin{aligned}
& \int_0^T \left\| \frac{d}{dt}C_R[u_C^R(t)] \right\|_{X_D} dt = \int_0^T \left\| C_R \left[ \frac{d}{dt}u_C^R(t) \right] \right\|_{X_D} dt \\
& = \int_0^T \sum_{i=1}^N i \left| \int_N^\infty a_R(y)b_i(y) \left[ \frac{d}{dt}u_C^R(t) \right](y) dy \right| dt \\
& \leq \alpha(R)N^2 \int_0^T \left\{ \int_N^\infty \left| \left[ \frac{d}{dt}u_C^R(t) \right](y) \right| y dy \right\} dt \\
& = \alpha(R)N^2 \int_0^T \left\| \frac{d}{dt}u_C^R(t) \right\|_{X_C} dt. \tag{6.25}
\end{aligned}$$

Recalling the abstract Cauchy problem (6.2), since the operators  $A_C^R$  and  $B_C^R$  are bounded and since  $u_C^R$  is given by a contraction semigroup, we have

$$\left\| \frac{d}{dt}u_C^R(t) \right\|_{X_C} \leq \|A_C^R + B_C^R\| \|u_C^R(t)\|_{X_C} \leq M \|c_0\|_{X_C},$$

where  $M$  is a constant such that  $\|A_C^R + B_C^R\| \leq M$ . Inserting this into (6.25) gives us

$$\int_0^T \left\| \frac{d}{dt}C_R[u_C^R(t)] \right\|_{X_D} dt \leq \alpha(R)N^2 \int_0^T M \|c_0\|_{X_C} ds \leq \alpha(R)N^2TM \|c_0\|_{X_C} < \infty.$$

Therefore the derivative of  $C_R[u_C^R(t)]$  belongs to the space  $L_1((0, T), X_D)$ ; hence, by Theorem 2.5.17, the equation (6.24) has a unique strong solution  $u_D^R : [0, T) \rightarrow X_D$ .  $\square$

Having established the existence of a unique strong solution to equation (6.24) given by (2.20), recalling Remark 2.5.18 this solution must also provide us with a unique mild solution to our equation. Now we consider the possibility of weak solutions, as defined in Definition 2.5.4. We aim to show that any weak solution of equation (6.24) must also be a mild solution (permitting changes on sets of measure zero), and hence the weak solution must be unique and differentiable.

**Theorem 6.2.3.** *Given an integrable weak solution  $u_D^R : [0, T) \rightarrow X_D$  of equation (6.24) as defined in Definition 2.5.4, then it must also be a strong solution. Therefore any integrable weak solution must be unique up to sets of measure zero and differentiable in  $X_D$ .*

*Proof.* Considering the right-hand side of equation (6.24), taking the norm in  $X_D$

and integrating from 0 to  $T$  gives us

$$\begin{aligned}
& \int_0^T \|(A_D + B_D)[u_D^R(t)] + C_R[u_C^R(t)]\|_{X_D} dt \\
& \leq \int_0^T \|(A_D + B_D)[u_D^R(t)]\|_{X_D} dt + \int_0^T \|C_R[u_C^R(t)]\|_{X_D} dt \\
& = \int_0^T \|(A_D + B_D)[u_D^R(t)]\|_{X_D} dt + \int_0^T \sum_{i=0}^N i \left| \int_N^\infty a_R(y) b_i(y) (u_C^R(t))(y) dy \right| dt \\
& \leq \int_0^T \|A_D + B_D\| \|u_D^R(t)\|_{X_D} dt + \alpha(R) N^2 \int_0^T \int_N^\infty |(u_C^R(t))(y)| y dy dt \\
& \leq \|A_D + B_D\| \int_0^T \|u_D^R(t)\|_{X_D} dt + \alpha(R) N^2 \int_0^T \|u_C^R(t)\|_{X_C} dt.
\end{aligned}$$

The assumption that  $u_D^R(t)$  is integrable and Theorem 2.2.10 allow us to deduce that the first of these integrals must be finite, whilst recalling that  $u_C^R(t)$  was given by a contraction semigroup immediately enables us to bound the second integral above. Hence, by Theorem 2.2.10, the right-hand side of equation (6.24) is integrable and therefore Theorem 2.5.6 tells us that the weak solution  $u_D^R(t)$  (allowing for changes on sets of measure zero) must also be a mild solution. Since, by Theorem 6.2.2, equation (6.24) has a unique mild solution which is in fact a strong solution, the weak solution  $u_D^R(t)$  we started with must agree with the strong solution (up to sets of measure zero) and therefore is unique and differentiable.  $\square$

Having established that any integrable weak solution of equation (6.24), in the sense of Definition 2.5.4, is also a strong solution, we now set out to prove that the solutions of equation (6.23) obtained in the previous chapter provide us with such a weak solution and in the process establish their uniqueness and differentiability.

**Lemma 6.2.4.** *The weak solutions  $u_{D_i}^R(t)$  to the equations (6.23), obtained from our numerical scheme in Chapter 5, when taken as the components of  $u_D^R : [0, T] \rightarrow X_D$ , produce a  $u_D^R$  which is integrable.*

*Proof.* The weak solutions  $u_{D_i}^R$  to the equations (6.23), constructed in the previous chapter, were obtained as the weak limits in  $L_1(0, T)$  of the sequences  $\{u_{D_i}^h\}$  as we let  $h \searrow 0$ . By the weak lower semicontinuity of the norm from Lemma 2.1.13 and using the bound (5.14), we obtain

$$\|u_{D_i}^R\|_{L_1(0, T)} \leq \liminf_{h \rightarrow 0} \|u_{D_i}^h\|_{L_1(0, T)} \leq CT,$$

where  $C$  denotes the constant from (5.14). If we take the components of the function  $u_D^R : [0, T] \rightarrow X_D$  to be given by  $u_{D_i}^R$  for  $i = 1, \dots, N$  then we get

$$\begin{aligned}
\int_0^T \|u_D^R(t)\|_{X_D} dt &= \int_0^T \sum_{i=1}^N i |u_{D_i}^R(t)| dt \leq N \sum_{i=1}^N \underbrace{\int_0^T |u_{D_i}^R(t)| dt}_{=\|u_{D_i}^R\|_{L_1(0, T)}} \leq N^2 CT < \infty.
\end{aligned}$$

Therefore the function  $u_D^R : [0, T] \rightarrow X_D$  formed by taking  $u_{D_i}^R$  as its  $i^{\text{th}}$  component is integrable.  $\square$

**Theorem 6.2.5.** *The weak solutions  $u_{D_i}^R : [0, T] \rightarrow \mathbb{R}$  for  $i = 1, \dots, N$  of the equations (5.16) obtained in the previous chapter agree with the components of the strong solution established in Theorem 6.2.2 and hence are unique (up to sets of measure zero) and differentiable.*

*Proof.* Let us consider our abstract equation (6.24) with the aim of rewriting it in a weak formulation as in (2.15). First let us note that the dual space of  $X_D$  is  $\mathbb{R}^N$  and the duality pairing  $\langle \cdot, \cdot \rangle$  appearing in (2.15) is given by the standard inner product on  $\mathbb{R}^N$ . Let  $u_D^R : [0, T] \rightarrow X_D$  be a weak solution of equation (6.24) with the components  $u_{D_i}^R : [0, T] \rightarrow \mathbb{R}$  for  $i = 1, \dots, N$ . Then, in this case, the function  $F : (0, T) \rightarrow X_D$  appearing in (2.15) is given componentwise by

$$F_i(t) = -a_i u_{D_i}^R(t) + \sum_{j=i+1}^N a_j b_{i,j} u_{D_j}^R(t) + \int_N^\infty a_R(y) b_i(y) (u_C^R(t))(y) dy,$$

for  $i = 1, \dots, N$ . Therefore the weak formulation of equation (6.24) becomes:

$$\begin{aligned} \sum_{i=1}^N \phi_i \int_0^T u_{D_i}^R(t) \frac{d}{dt} \psi(t) dt &= - \sum_{i=1}^N \phi_i d_{0i} \psi(0) + \sum_{i=1}^N \phi_i \int_0^T a_i u_{D_i}^R(t) \psi(t) dt \\ &- \sum_{i=1}^N \phi_i \int_0^T \sum_{j=i+1}^N a_j b_{i,j} u_{D_j}^R(t) \psi(t) dt - \sum_{i=1}^N \phi_i \int_0^T \int_N^\infty a_R(y) b_i(y) u_C^R(y, t) \psi(t) dy dt, \end{aligned}$$

for any  $\phi = (\phi_1, \dots, \phi_N) \in \mathbb{R}^N$  and  $\psi \in C_c^\infty([0, T])$ , where  $u_C^R(\cdot, t)$  is the (unique) real-valued representation of the  $X_C$ -valued  $u_C^R : [0, T] \rightarrow X_C$ .

Comparing this with equation (5.16) of the previous chapter it is easily seen that the  $u_{D_i}^R$  obtained there provide us with a solution to the above equation and so taking these  $u_{D_i}^R : [0, T] \rightarrow \mathbb{R}$ ,  $i = 1, \dots, N$ , as the components of an  $X_D$ -valued function  $u_D^R : [0, T] \rightarrow X_D$  provides us with an integrable weak solution to equation (6.24). As any such  $u_D^R : [0, T] \rightarrow X_D$  must be unique and differentiable in  $X_D$ , the components  $u_{D_i}^R : [0, T] \rightarrow \mathbb{R}$  must be unique (up to sets of measure zero) and differentiable in the traditional sense.  $\square$

Having established the tie between the solutions of the truncated inhomogeneous abstract Cauchy problem (6.24) and the numerically obtained weak solutions of (5.16) from the previous chapter, we now look to let  $R \rightarrow \infty$  and show that the solution  $u_D^R$  of the truncated equation (6.24) converges to the solution  $u_D$  of the non-truncated equation (3.17) from Chapter 3.

**Theorem 6.2.6.** *Under the assumptions made so far, the sequence of truncated solutions  $\{u_D^R\}$  converges strongly to the full solution  $u_D$  in  $X_D$  as  $R \rightarrow \infty$ .*

*Proof.* Using the formula (2.20) for both  $u_D^R$  and  $u_D$ , we get for  $t \in [0, T)$  that

$$\begin{aligned}
\|u_D^R(t) - u_D(t)\|_{X_D} &= \left\| \int_0^t T(t-s) (C_R[u_C^R(s)] - C[u_C(s)]) \, ds \right\|_{X_D} \\
&\leq \int_0^t \|T(t-s)\| \|C_R[u_C^R(s)] - C[u_C(s)]\|_{X_D} \, ds \\
&\leq M' e^{\omega|t} \int_0^t \|C_R[u_C^R(s)] - C[u_C(s)]\|_{X_D} \, ds \\
&\leq M' e^{\omega|T} \int_0^T \|C_R[u_C^R(s)] - C[u_C(s)]\|_{X_D} \, ds, \tag{6.26}
\end{aligned}$$

where  $M'$  and  $\omega$  are constants such that a bound of the form (2.9), from Theorem 2.4.3, holds for our semigroup  $(T(t))_{t \geq 0}$ . Considering the integrand from (6.26) more carefully, we can see that

$$\begin{aligned}
&\|C_R[u_C^R(s)] - C[u_C(s)]\|_{X_D} \\
&= \sum_{i=1}^N i \left| \int_N^\infty b_i(y) (a_R(y)[u_C^R(s)](y) - a(y)[u_C(s)](y)) \, dy \right| \\
&\leq \int_N^\infty \left( \sum_{i=1}^N i b_i(y) \right) a(y) |[u_C^R(s)](y) - [u_C(s)](y)| \, dy \\
&= \int_N^\infty \left( y - \int_N^y x b(x|y) \, dx \right) a(y) |[u_C^R(s)](y) - [u_C(s)](y)| \, dy \\
&= c (|u_C^R(s) - u_C(s)|), \tag{6.27}
\end{aligned}$$

where  $c$  is the functional defined in Theorem 3.2.2 and where condition (3.3) has been utilised to obtain  $c$  here. Recalling that  $u_C^R(s)$  is given in  $X_C$  by  $S_R(s)c_0^R$ , which by (6.10) yields

$$u_C^R(s) = S_R(s)c_0^R = \bar{T}_R(s)c_0.$$

From Theorems 6.1.8 and 6.1.10, we also have

$$u_C(s) = G_K(s)c_0 = G(S)c_0 = \lim_{R \rightarrow \infty} \bar{T}_R(s)c_0.$$

The increasing nature of the family of  $(\bar{T}_R(t))_{t \geq 0}$ , established in Lemma 6.1.6, then allows us to deduce

$$u_C(s) = \lim_{R \rightarrow \infty} \bar{T}_R(s)c_0 \geq \bar{T}_R(s)c_0 = u_C^R(s),$$

hence

$$|u_C^R(s) - u_C(s)| = u_C(s) - u_C^R(s).$$

As per Lemma 6.1.7, we know that  $u_C^R(s) \in D(K)$ , whilst since  $u_C$  is generated by  $K$ , it is a standard result (Theorem 2.4.11) that  $u_C(s) \in D(K)$  for all  $s \geq$

0. Therefore, we have  $u_C(s) - u_C^R(s) \in D(K)$ , for all  $s \geq 0$ . Furthermore, by Theorem 6.1.8,  $u_C^R(s) \rightarrow u_C(s)$  in  $X_C$ , with the convergence being uniform with respect to  $s$  on bounded intervals. Since, by Lemma 2.5.25,  $c$  is a continuous linear functional on  $D(K)$  we have

$$c(|u_C^R(s) - u_C(s)|) = c(u_C(s) - u_C^R(s)) \rightarrow 0,$$

with the convergence again being uniform with respect to  $s$  on bounded intervals. In combination with (6.27) and (6.26), this uniform convergence allows us to deduce that the sequence of truncated solutions  $\{u_D^R\}$  converges to the full solution  $u_D$  in  $X_D$  as  $R \rightarrow \infty$ . □

*Remark 6.2.7.* We note that in [56], a fully discrete fragmentation model was examined in a weighted  $\ell_1$  space via the Kato–Voigt perturbation theorem (Theorem 2.5.22) and (an extension of) the fragmentation operators were found to generate a substochastic semigroup (Definition 2.4.4). We can think of infinitely extending our finite discrete fragmentation operators  $A_D$  and  $B_D$  by zero to form truncated operators in the  $\ell_1$  space of [56]. This extension exercise forms an isometry between our discrete space  $X_D$  and a truncation subspace of the weighted  $\ell_1$  space, as such the norms of the operators and the semigroup they generate would agree between spaces. Since the semigroup in [56] was substochastic, we can therefore take  $M'$  and  $\omega$  above to be 1 and 0 respectively. Taking account of this, the obvious substitution of the inequality (6.27) into (6.26) leads to the following bound, which holds for  $t \in [0, T]$ :

$$\begin{aligned} \|u_D^R(t) - u_D(t)\|_{X_D} &\leq \int_0^T c(|u_C^R(s) - u_C(s)|) \, ds \\ &\leq k_c \int_0^T \|u_C(s) - u_C^R(s)\|_{X_C} \, ds, \end{aligned}$$

where  $k_c$  denotes the bound on the functional  $c$  taken over  $D(K)$ . Hence the error within the discrete regime due to the truncation of the continuous mass interval, is determined in large part by the truncation error within the continuous regime. We shall return to this point in the following chapter, when we experimentally examine the convergence as  $R \rightarrow \infty$ .

In this chapter we completed the tie-up between the numerical weak solutions, considered over the preceding chapters, and the strong analytic solutions established in Chapter 3. By relating the scalar-valued weak formulation of our truncated equations to an equivalent weak formulation within a Banach space setting, we were able to establish a one-to-one relationship between the associated scalar and Banach-space-valued weak solutions. Under suitable constraints, these Banach space weak solutions were shown to be the unique strong solutions and hence

our original scalar weak solutions must also be unique. Additionally, as a further consequence of this tie up, the scalar weak solutions were shown to be differentiable classical solutions. Finally, we considered letting the truncation parameter  $R$  go to infinity. In doing so, the strong solutions of the truncated Banach space evolution equation were shown to converge to the solution provided by the semi-group in Chapter 3, completing the link between our numerical solutions and those established via analytic means.

# Chapter 7

## Numerical Experimentation

In this chapter we shall apply the numerical scheme developed in Chapter 4 to a selected class of test models. The models selected are chosen partly due to the widespread consideration given in the literature to the analogous continuous models, and partly the availability of exact solutions, allowing for an assessment of the efficacy of our scheme. However prior to this we shall briefly investigate a degenerate case of the standard continuous fragmentation model, (1.5), aiming to demonstrate the phenomenon of shattering.

### 7.1 Continuous Fragmentation Model: A Demonstration of Shattering

We start by considering the continuous multiple fragmentation equation, with power law kernels, as given by (1.5) and (1.7). More specifically, we shall be considering the case of binary fragmentation ( $\nu = 0$ ) as modelled by the following equation:

$$\frac{\partial u(x, t)}{\partial t} = -x^\alpha u(x, t) + 2 \int_x^\infty y^{\alpha-1} u(y, t) dy, \quad x > 0, t > 0, \quad (7.1)$$

where  $\alpha \in \mathbb{R}$ . The more general form of this model, was considered by McGrady and Ziff in [57], under the assumption of a mono-disperse initial condition, that is  $u(x, 0) = \delta(x - l)$ ,  $l > 0$ , and found to display mass loss through ‘shattering’ in cases where  $\alpha < 0$ . Using a Laplace transform method, Huang, Edwards and Levine [37], provided an explicit solution to the multiple fragmentation equation from (1.5) and (1.7). For the case of  $\alpha = -1$  and  $\nu = 0$  ( $\alpha = -1$  in (7.1)), the solution provided in [37] reduces to

$$u(x, t) = e^{-t/x} u(x, 0) + \int_x^\infty y^{-2} e^{-t/y} \left( 2t + t^2 \left( \frac{1}{x} - \frac{1}{y} \right) \right) u(y, 0) dy, \quad (7.2)$$

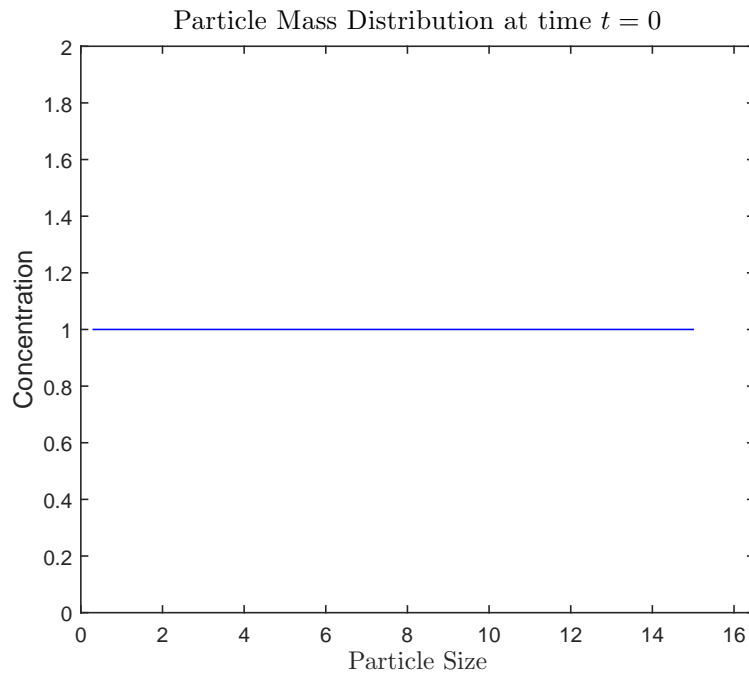
where  $x > 0$  and  $t \geq 0$ . Let us impose the following truncated uniform initial state:

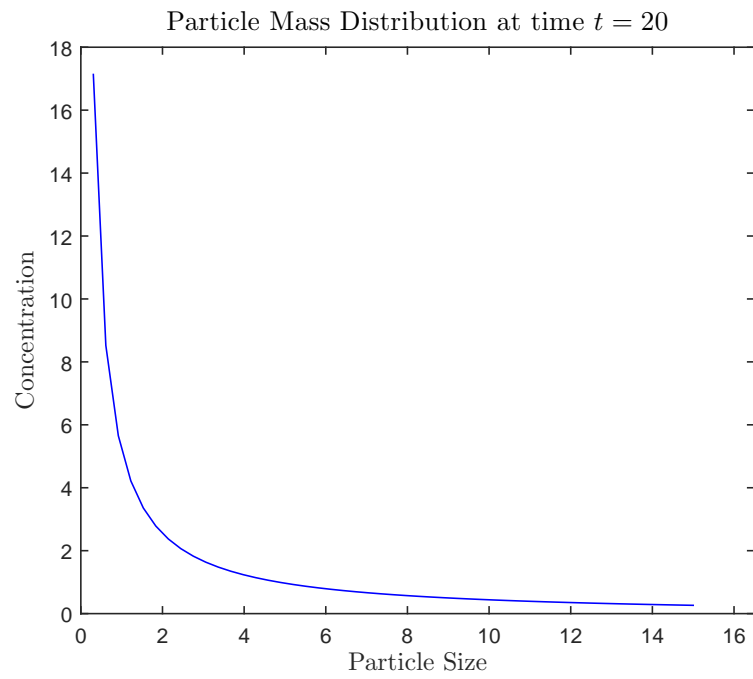
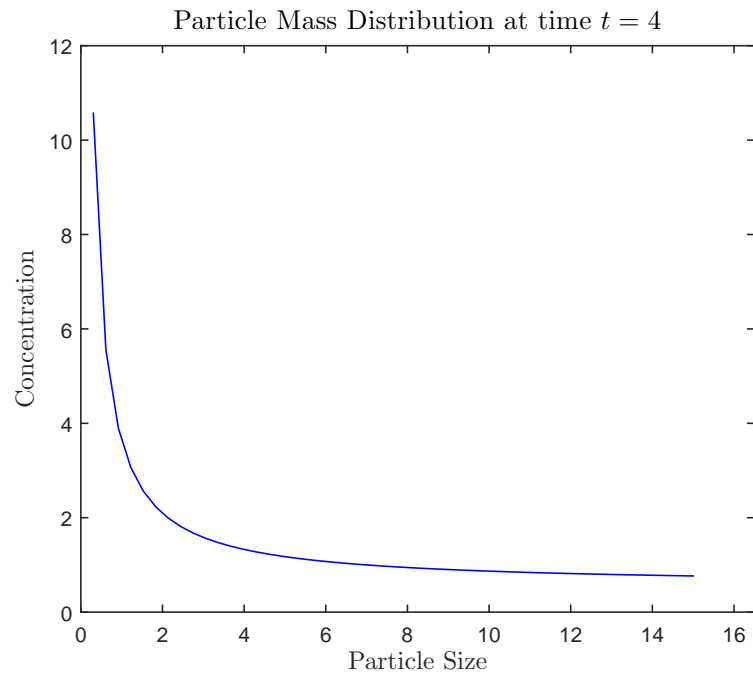
$$u(x, 0) = \begin{cases} 1 & \text{for } 0 < x < R, \\ 0 & \text{for } x \geq R, \end{cases}$$

where  $R > 0$  is a constant; then the solution given in (7.2), can be evaluated to give

$$u(x, t) = e^{-t/R} \left( 1 + t \left( \frac{1}{x} - \frac{1}{R} \right) \right), \quad \text{for } 0 < x < R, \quad (7.3)$$

and  $u(x, t) = 0$  for  $x \geq R$ . As an example, to demonstrate how the mass distribution evolves with time under this model, below are a number of plots of (7.3) in the case of  $R = 15$  at a range of values for  $t$ .





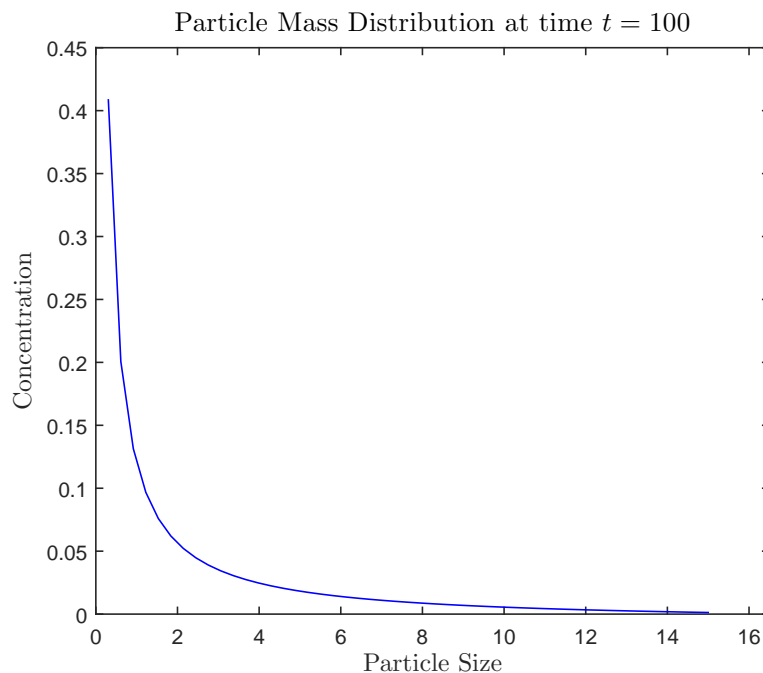


Figure 7.1: Particle mass distribution at time  $t = 0, 4, 20$  and  $100$ .

As one might expect from consideration of the physical process we are modelling, as time evolves and particles fragment, the mass becomes increasingly concentrated amongst the smaller particles, resulting in a peak on the left side of our charts. However, a closer examination of the  $y$ -axis scales between the charts for  $t = 20$  and  $t = 100$  points to the problem we are seeking to address. If we integrate the density  $u(x, t)$  over the positive real line with respect to the measure  $x dx$ , then we obtain the total mass,  $M(t)$ , within the system at time  $t$ . Doing so for (7.3) yields

$$M(t) = \frac{1}{2}R(R + t)e^{-t/R}. \quad (7.4)$$

Computing this quantity against time for the case described above, we can observe a loss in the total mass, as seen from Figure 7.2. This agrees with the results of McGrady and Ziff from [57], where the process leading to the loss was termed ‘shattering’ and attributed to the loss of mass to ‘zero’-size particles.

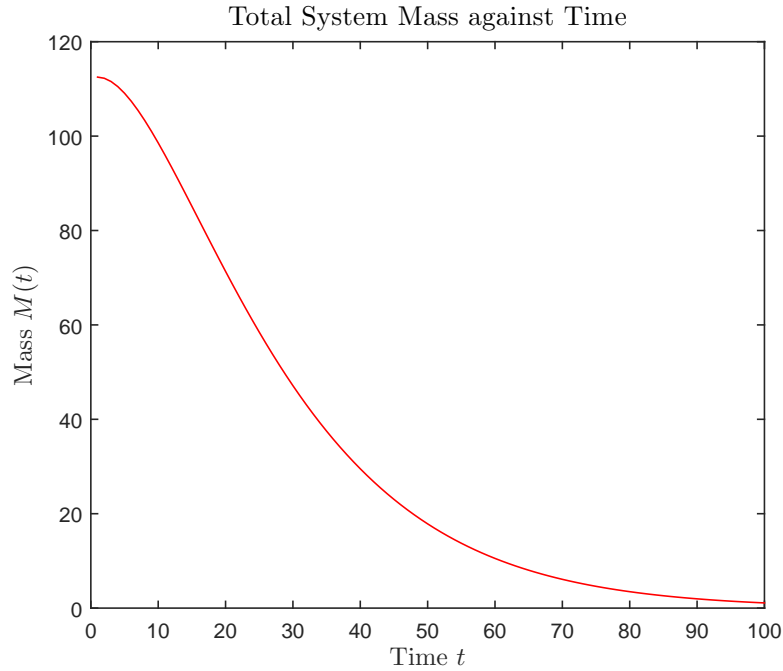


Figure 7.2: Total system mass through time.

## 7.2 Mixed Discrete–Continuous Test Model

The concept of a hybrid discrete–continuous model, as developed in this thesis, was proposed as a solution to this ‘shattering’ mass loss. We shall now introduce a particular class of such models, to which, we will go on to apply the numerical scheme from Chapter 4. The model is based upon the power law fragmentation model, given by (1.7). For our investigation, the continuous regime equation (3.1), will therefore be specified by

$$a(x) = x^\alpha, \quad \alpha \in \mathbb{R}, \quad \text{and} \quad b(x|y) = (\nu + 2) \frac{x^\nu}{y^{\nu+1}}, \quad -2 < \nu \leq 0, \quad (7.5)$$

for  $N < x \leq y$ . With this model selection, our continuous regime equation becomes

$$\frac{\partial u_C(x, t)}{\partial t} = -x^\alpha u_C(x, t) + (\nu + 2)x^\nu \int_x^\infty y^{\alpha-\nu-1} u_C(y, t) dy, \quad x > N, \quad t > 0. \quad (7.6)$$

The analogous purely continuous model corresponds to the class to which our earlier example model belongs. This class was considered by McGrady and Ziff in [57] and found to display mass loss through ‘shattering’ in the case that  $\alpha < 0$ , as demonstrated above.

Moving on to the discrete regime equation, (3.2), in specifying our discrete regime equation we must provide a set of continuous to discrete mass distribution functions  $b_i(y)$ ,  $i = 1, \dots, N$ , such that condition (3.3) is satisfied. If we take these functions to be given by

$$b_i(y) = \frac{i^{\nu+2} - (i-1)^{\nu+2}}{iy^{\nu+1}}, \quad y > N, \quad i = 1, \dots, N, \quad (7.7)$$

where the value of  $\nu$  is the same as in (7.5) and (7.6), then it is easily verified that condition (3.3) is satisfied.

Finally we must specify a choice for the discrete fragmentation parameter values  $a_i$  and  $b_{i,j}$ , where the  $b_{i,j}$  must satisfy (3.4). There are a number of different choices for these values considered in the literature. However, for our model we shall take the case of uniform binary fragmentation, whereby two particles are produced from each fragmentation event, and all admissible pairings of resulting particle sizes are equally likely. This is obtained by setting

$$b_{i,j} = \frac{2}{j-1}, \quad i = 1, \dots, N-1, \quad j = i, \dots, N.$$

Primarily we have selected this particular model for its simplicity, however versions of this model were studied in [75], one of the earliest articles on discrete fragmentation, and also in the paper [84].

When it comes to the selection of the values  $a_i$ , there are minimal restrictions which must be satisfied and we can largely select any non-negative values we wish. However, whereas  $a_i = 1$ , was selected in [75] and  $a_i = (i-1)/(i+1)$ , in [84], we shall take

$$a_i = i^\alpha, \quad i = 2, \dots, N,$$

with  $a_1 = 0$ , in order to mirror the choice for the continuous fragmentation rate  $a(x)$ . Taking these selections leads to the following set of equations for the discrete regime:

$$\frac{du_{Di}(t)}{dt} = -i^\alpha u_{Di}(t) + \sum_{j=i+1}^N \frac{2j^\alpha}{j-1} u_{Dj}(t) + \frac{i^{\nu+2} - (i-1)^{\nu+2}}{i} \int_N^\infty y^{\alpha-\nu-1} u_C(y, t) dy, \quad (7.8)$$

for  $i = 1, \dots, N$  and  $t > 0$ , where we lose the  $-i^\alpha u_{Di}(t)$  term for  $i = 1$  and the summation term disappears for  $i = N$ .

## 7.3 Mixed Model Numerical Solution Examples

### 7.3.1 Example Model 1 ( $\alpha = -1$ and $\nu = 0$ )

Taking the model introduced in the previous section, we examine the particular case of  $\alpha = -1$  and  $\nu = 0$ . Taking such a choice of parameters in the standard continuous model has been shown to result in a shattering process [57], and numerically demonstrated in the previous section. As a preliminary investigation of the behaviour of our model and numerical scheme, we ran the Matlab code implementation `numfrag.m`, given in Appendix B, with the parameters  $N = 5$ ,  $R = 15$ , discretising the continuous mass interval using,  $I_h = 20$ , equal length intervals. We set the end time  $T$  equal to 100, to give sufficient time for the system to settle to its equilibrium, and discretised the time interval with  $M = 25$  intervals of equal length. Starting with a uniform initial mass distribution where  $d_{0i} = 1$  for  $i = 1, \dots, 5$  and  $c_0(x) = 1$ , we observed the behaviour displayed in the following figures.

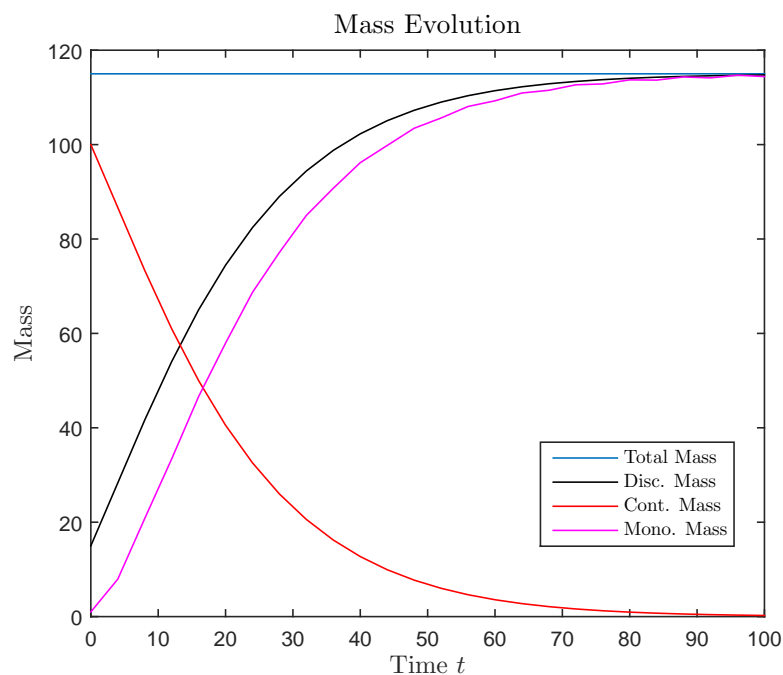


Figure 7.3: The evolution of masses with time.

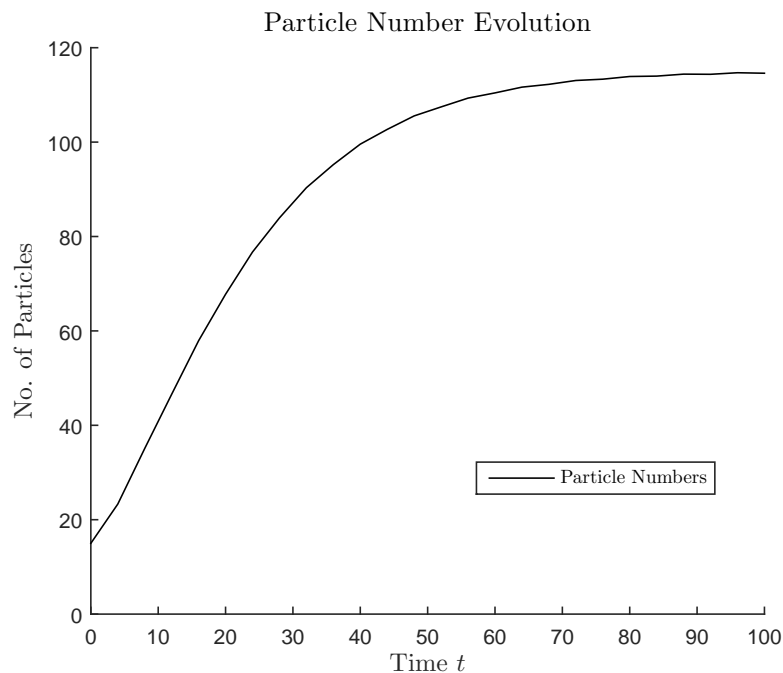
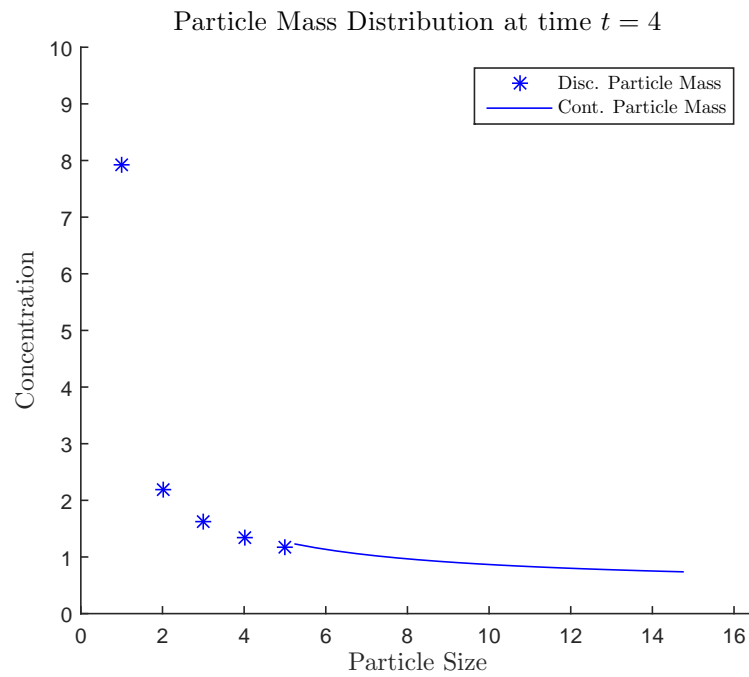
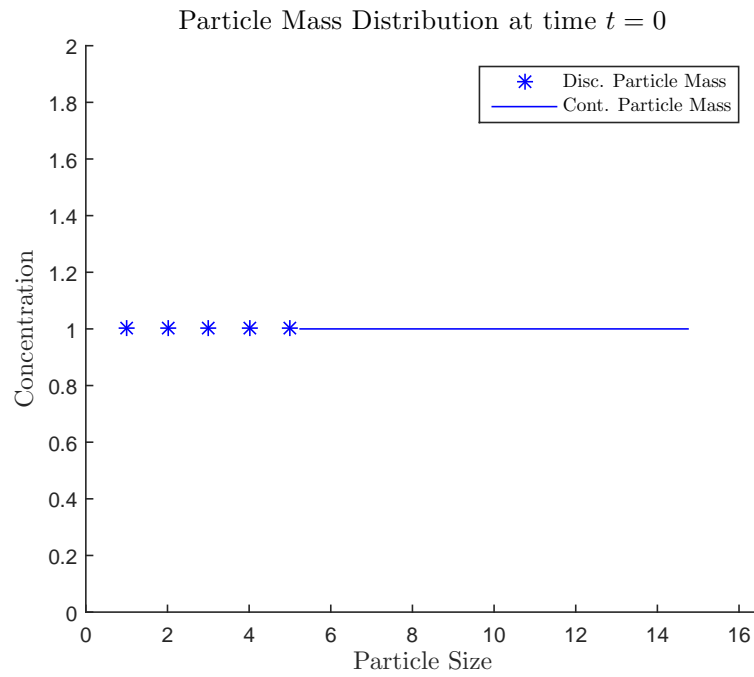


Figure 7.4: The evolution of particle numbers with time.

Figure 7.3 details the evolution of the total mass (blue), along with the mass accounted for by the continuous regime (red), the total mass within the discrete regime (black) and the total mass accounted for by monomers (magenta). As we would hope, the total mass within the system remains constant, with a reduction in the continuous regime total mass being balanced by a gain in the total mass of the discrete regime, resulting from the fragmentation of larger continuous mass particles into smaller discrete mass particles. As time evolves, the mass accounted for by monomers grows to form an ever larger proportion of the total mass, until we reach a stage where they constitute the vast majority of the total mass and the system approaches an equilibrium. This behaviour is supported by Figure 7.4, which details the evolution of the particle numbers within the system. Initially we see a rapid increase in the total number of particles, as particles of all masses greater than one fragment producing further particles. However as monomers come to dominate the particle size distribution then the growth in numbers slows, leveling off as we approach the equilibrium.



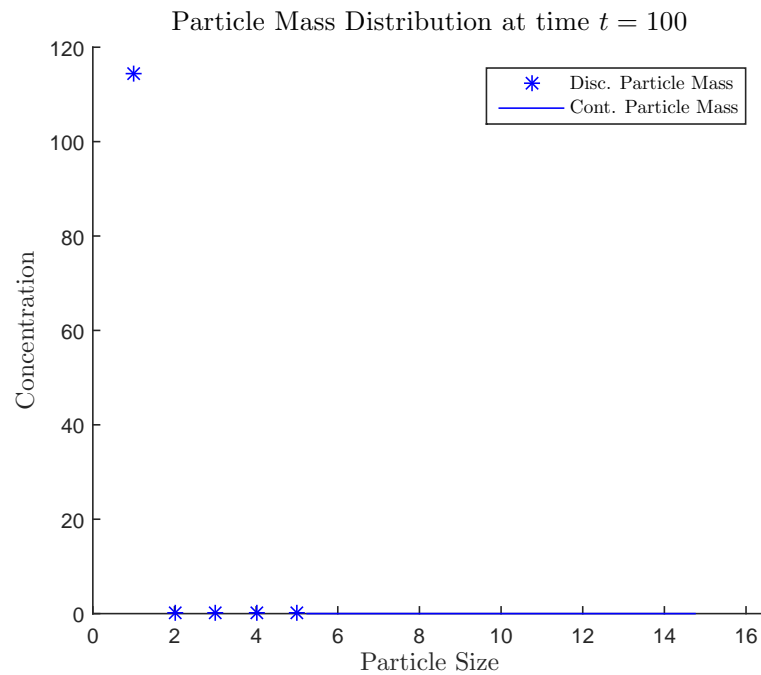
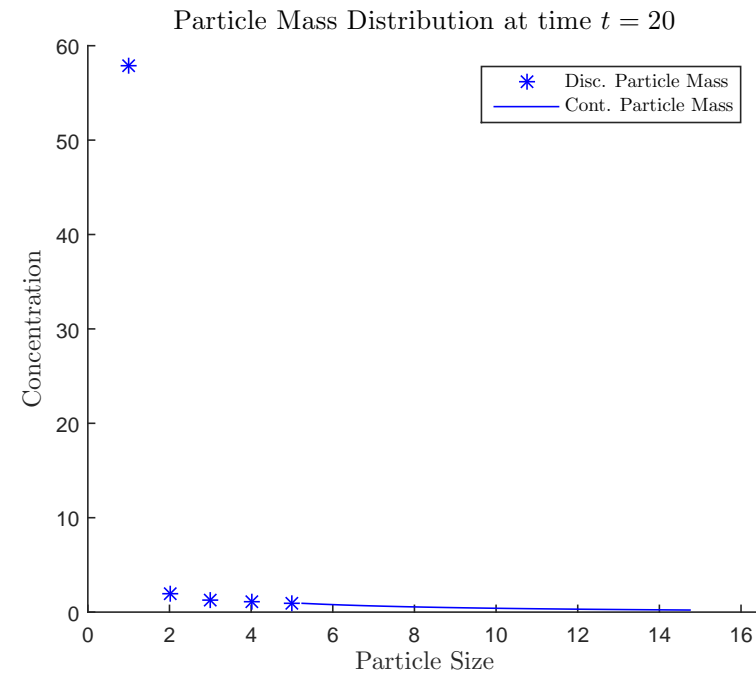


Figure 7.5: Particle mass distribution at time  $t = 0, 4, 20$  and  $100$ .

Above can be seen a selection of charts depicting the evolution of the mass distribution through time, starting in the uniform initial state through to the final

equilibrium state. In these charts, we have graphed the continuous regime by attributing the approximating value over each interval to the interval midpoint, then plotting through these points using the Matlab `plot` command.

### 7.3.2 Example Model 2 ( $\alpha = 0.5$ and $\nu = -0.5$ )

In order to investigate the model behaviour and whether it fits with our physical intuition regarding the system, we vary the model parameters and observe the effect on the computed solutions. This also allows us to assess the performance of our numerical scheme under a range of conditions. In this case we will set  $\alpha = 0.5$  and  $\nu = -0.5$ , which has the effect of increasing the fragmentation rate and changing the resulting size distribution for fragmentation events, to favour smaller particles. We would expect both of these changes to speed up the fragmentation process, and for equilibrium to be reached quicker than in the previous case. As before, we ran the Matlab code `numfrag.m` with  $N = 5$ ,  $R = 15$  and  $I_h = 20$  equal length intervals for the mass variable.

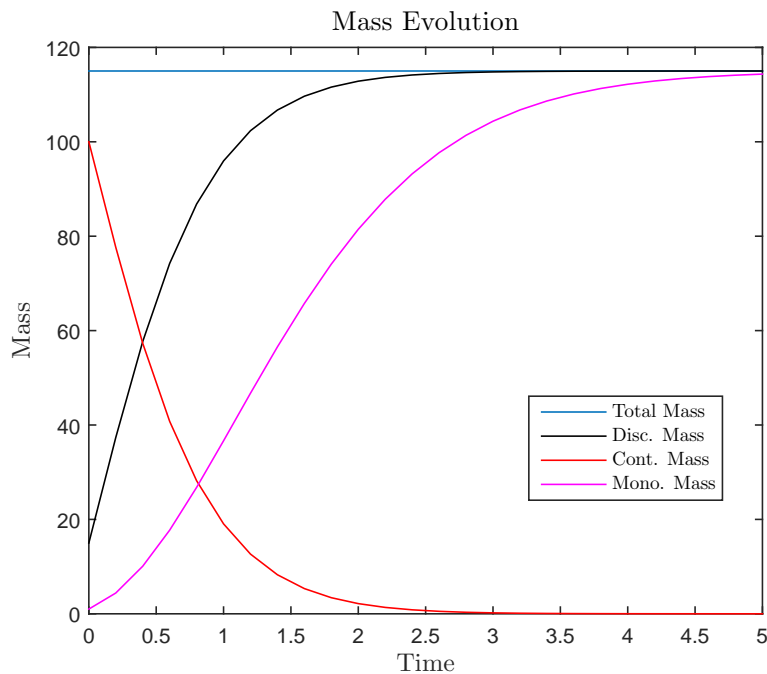


Figure 7.6: The evolution of masses with time.

The approximation was run with a termination time of  $T = 5$ , discretised using  $M = 20$  intervals of equal length, to give the charts in Figure 7.6. As before, we see that the total mass (blue) is conserved with the loss from the continuous regime (red) being balanced by an increase in the discrete regime (black). However if we compare the model behaviour to that observed in Figure 7.3, we see that the process reaches an equilibrium state significantly quicker than in the previous case,

as expected from an intuitive consideration of the model setup. Additionally we note that the time mesh taken here is finer than that employed with Model 1; this was required in order to ensure that the solutions remained non-negative. This is consistent with Lemma 4.3.1, as the bounds listed there are reduced by the changes made here, suggesting a smaller time-step is required.

## 7.4 Mixed Model Exact Solutions and Performance of Numerical Scheme

As stated earlier, the particular model introduced in Section 7.2 was chosen partly due to the availability of exact solutions which enables an assessment of the accuracy of our numerical method. Here we will detail how these exact solutions may be obtained.

### 7.4.1 Exact Solutions

The continuous regime equation (7.6), coincides with the one provided for the ‘fragmentation state’ in [38, Section 3]. When this equation is coupled with an initial continuous mass distribution  $c_0(x)$ , then [38, Equation (9)] gives the solution as

$$u_C(x, t) = e^{-x^\alpha t} \left\{ c_0(x) + m \alpha t x^\nu \int_x^\infty y^{\alpha-\nu-1} c_0(y) {}_1F_1(1-m, 2, t(x^\alpha - y^\alpha)) dy \right\}, \quad (7.9)$$

where  $m = (2 + \nu)/\alpha$  and  ${}_1F_1$  is the confluent hypergeometric function given by

$${}_1F_1(a, b, z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)} \frac{\Gamma(b)}{\Gamma(b+n)} \frac{z^n}{n!}.$$

To solve the set of discrete regime equations (7.8), we write them as the system

$$\frac{d}{dt} \underline{u}_D(t) = C \underline{u}_D(t) + \underline{F}(t), \quad (7.10)$$

where  $\underline{u}_D(t) = (u_{D1}(t), \dots, u_{DN}(t))^T$ , the  $N \times N$  matrix  $C$  has the entries

$$c_{i,j} = \begin{cases} 0 & \text{for } i = j = 1 \text{ or } i > j, \\ -i^\alpha & \text{for } i = j > 1, \\ \frac{2j^\alpha}{j-1} & \text{for } j > i, \end{cases}$$

and where  $\underline{F} : [0, \infty) \rightarrow \mathbb{R}^N$  has the components

$$F_i(t) = \underbrace{\frac{i^{\nu+2} - (i-1)^{\nu+2}}{i}}_{\beta_i(\nu)} \int_N^\infty y^{\alpha-\nu-1} u_C(y, t) dy, \quad (7.11)$$

for  $i = 1, \dots, N$ , and  $u_C(y, t)$  given by (7.9). When the initial state of the vector  $\underline{u}_D(t)$  is  $d_0$ , then the system (7.10) has the solution

$$\underline{u}_D(t) = e^{Ct} \left\{ d_0 + \int_0^t e^{-sC} \left( \int_N^\infty y^{\alpha-\nu-1} u_C(y, s) dy \right) ds \underline{\beta}(\nu) \right\}, \quad (7.12)$$

where  $\underline{\beta}(\nu)$  is the vector of values  $(\beta_1(\nu), \dots, \beta_N(\nu))^T$  from (7.11), and  $e^M$  denotes the matrix exponential of a matrix  $M$ .

The Matlab code `exactfrag.m`, which may be found in Appendix B, evaluates the solutions (7.9) and (7.12) at the same gridpoints as the numerical code `numfrag.m`.

## 7.4.2 Numerical Performance

To assess the efficacy of our numerical scheme, we tested it on the model introduced in Section 7.2. The approximate solutions generated were compared to the exact solutions derived in the previous section, with the discrepancy being measured by taking the relative error with respect to the norm on  $L_1([0, T], X_D) \times L_1([0, T], X_C)$ . That is, supposing  $u^h = (\underline{u}_D^h(t), u_C^h(x, t))$  is our approximation of an exact solution  $u = (\underline{u}_D(t), u_C(x, t))$ , then we measure the error via

$$Error(u^h|u) = \frac{\|u^h - u\|}{\|u\|}, \quad (7.13)$$

where the norm  $\|\cdot\|$ , is given by

$$\begin{aligned} \|u\| &= \int_0^T \|\underline{u}_D(t)\|_{X_D} dt + \int_0^T \|u_C(\cdot, t)\|_{X_C} dt \\ &= \int_0^T \sum_{i=1}^N i |u_{Di}(t)| dt + \int_0^T \int_N^\infty |u_C(x, t)| x dx dt. \end{aligned} \quad (7.14)$$

Imposing an initial state, with

$$c_0(x) = \begin{cases} 1 & \text{for } N < x < R, \\ 0 & \text{for } x \geq R, \end{cases}$$

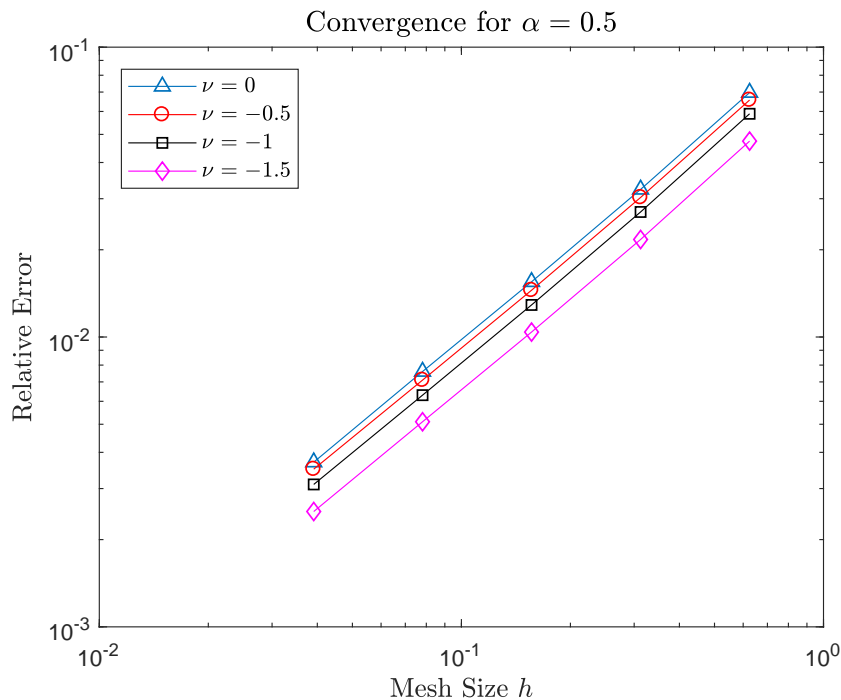
and  $d_0$  being the  $N$ -vector consisting entirely of 1's, a range of numerical experiments were conducted. The parameters  $\alpha$  and  $\nu$  were varied, taking all possible combinations of  $\alpha \in \{0.5, 0.1, -0.5, -1, -2\}$  and  $\nu \in \{0, -0.5, -1, -1.5\}$ . The parameters  $N$  and  $R$  were, for the time being, held at 5 and 15 respectively and in all cases  $T$  was selected to allow the system to reach a near equilibrium state. Our approximate solutions were, once again, computed using the Matlab code `numfrag.m`, over a range of meshes. The exact solution was evaluated using the code `exactfrag.m`; this was carried out on a fine mesh, chosen in such a way as to

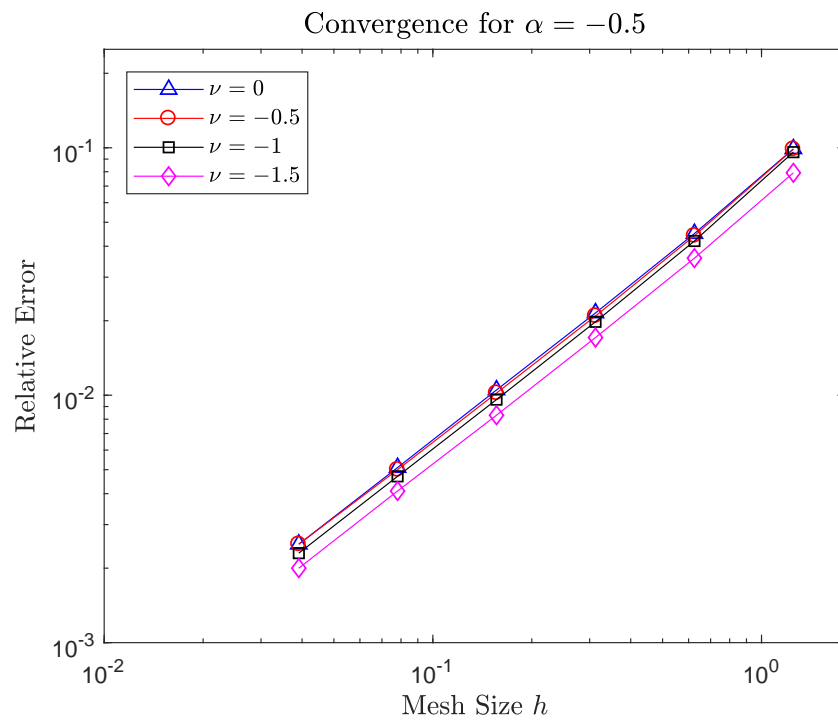
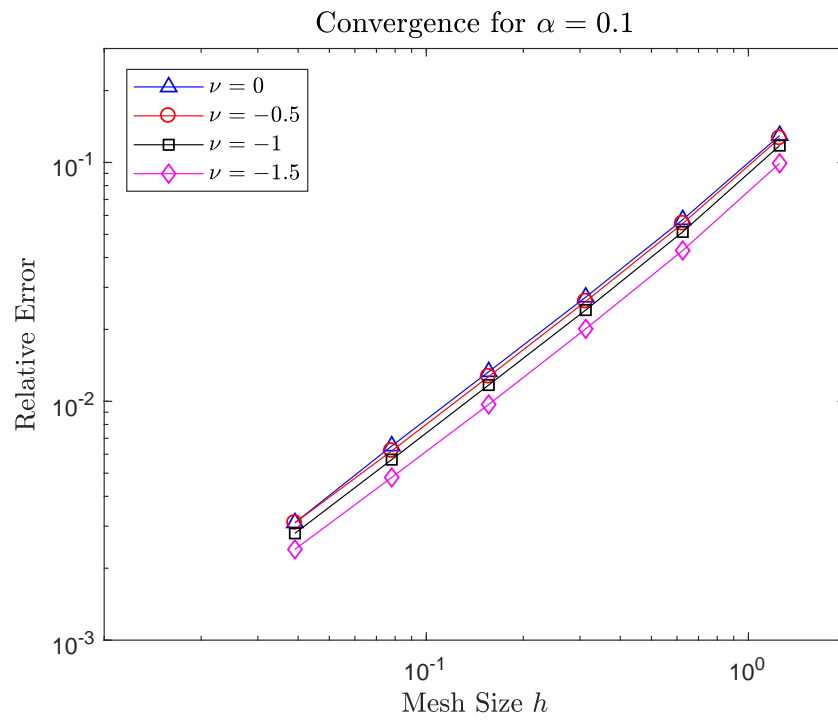
be a refinement of each of the meshes used for the approximations. The integrals in the error (7.13) were then approximated using the rectangle rule, implemented via the Matlab code `numerror.m`. As an example, we have included the results for the parameter choices  $\alpha = 0.5$  and  $\nu = 0$  below. The full results for all experimental configurations may be found together, for ease of comparison, at the end of this thesis in Appendix A.

Parameters: $N = 5, R = 15, T = 6, \alpha = 0.5, \nu = 0,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 5.8594 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	0.62500	0.18750	$6.9714 \times 10^{-2}$	NA
2	0.31250	$9.3750 \times 10^{-2}$	$3.2251 \times 10^{-2}$	1.1121
3	0.15625	$4.6875 \times 10^{-2}$	$1.5508 \times 10^{-2}$	1.0563
4	$7.8125 \times 10^{-2}$	$2.3438 \times 10^{-2}$	$7.5624 \times 10^{-3}$	1.0361
5	$3.9063 \times 10^{-2}$	$1.1719 \times 10^{-2}$	$3.7215 \times 10^{-3}$	1.0229

Table 7.1: Experimental results for the case  $\alpha = 0.5$  and  $\nu = 0$ . The values of  $\gamma_{n-1}$  relate to the order of convergence, the definition of which is given in the upcoming section (page 135).

From even the briefest examination of the data in Appendix A, it is clear that as the mesh is refined, the relative error of the approximations is reduced. This can also be seen from the following charts, which plot mesh size  $h$  against relative error for each of the model scenarios examined.





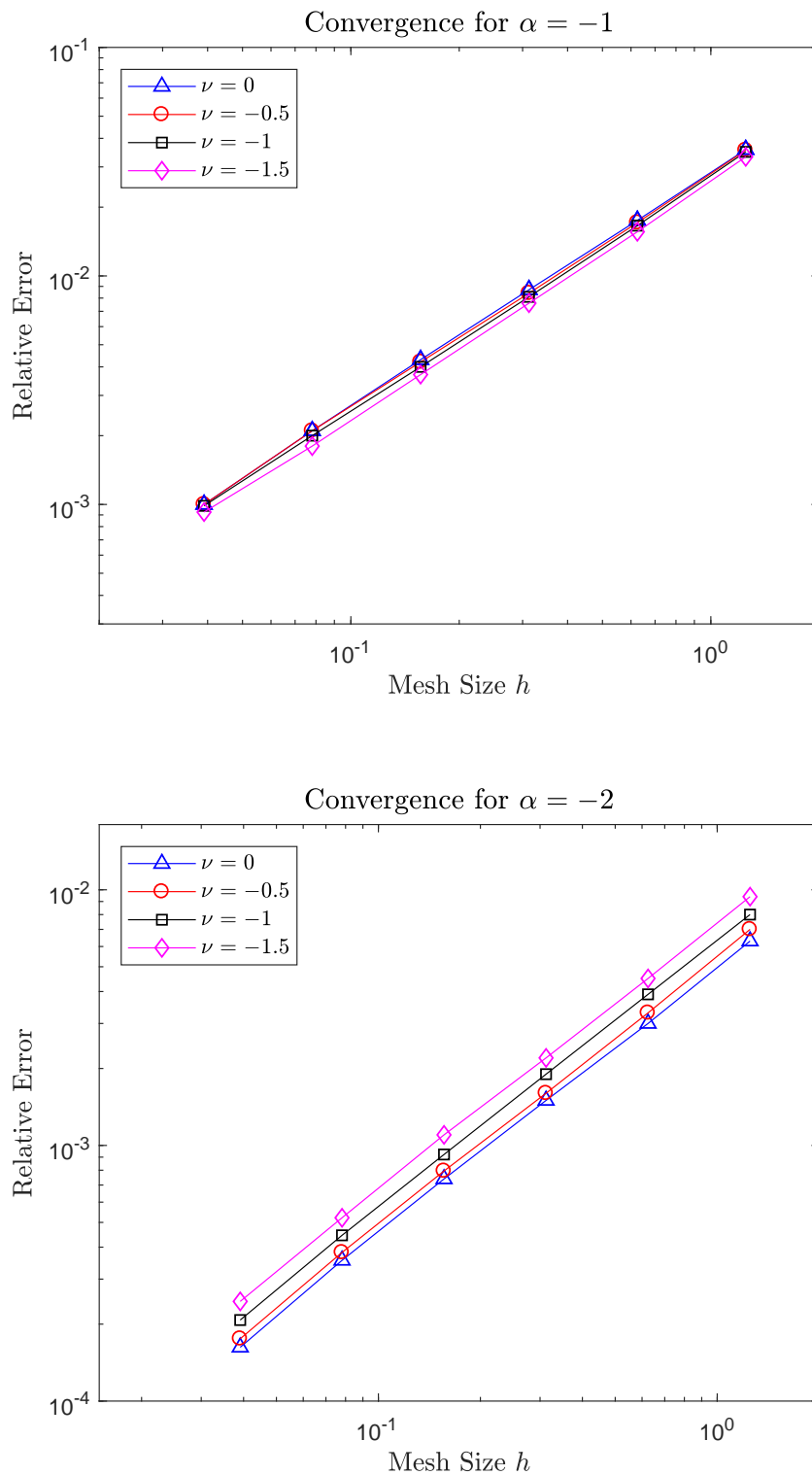


Figure 7.7: Numerical convergence for  $\alpha = 0.5, 0.1, -0.5, -1$  and  $-2$ . The errors in the case of  $\alpha = -2$  were calculated against a numerical approximation, computed on a fine mesh, in place of an exact solution.

### Order of Convergence

It would seem clear from the evidence presented thus far that the approximations do indeed improve as we refine the mesh upon which they are based. However, we are interested in quantifying this relationship and gaining an indication on the extent of the improvement we might expect, given a refinement of our mesh.

Let us imagine an approximation based on a mesh with size parameter  $h$  and with associated error  $E$ ; then we might postulate that the error is related to the mesh size in the following manner:

$$E \sim Ch^\gamma, \quad \text{as } h \rightarrow 0^+, \quad (7.15)$$

where  $C$  and  $\gamma$  are constants. This being the case, we refer to  $\gamma$  as the *order of convergence*, and generally the greater the value of  $\gamma$  the better. As far as determining the order in practice, we proceed as follows. Suppose we have a sequence of approximations based on meshes with the size parameters  $\{h_k\}_{k=1}^\infty$ , where  $h_{k+1} < h_k$  and let  $\{E_k\}_{k=1}^\infty$  denote the sequence of associated errors, then successive approximations should satisfy the relation (7.15). Taking a ratio for successive errors yields

$$\frac{E_{n+1}}{E_n} \sim \left( \frac{h_{n+1}}{h_n} \right)^\gamma.$$

Assuming that the mesh has been refined in a regular manner so that for all  $n$  we have  $h_{n+1} = \frac{1}{m}h_n$ , for some integer  $m$ , then the previous relation becomes

$$\frac{E_{n+1}}{E_n} \sim \left( \frac{1}{m} \right)^\gamma = m^{-\gamma}.$$

Taking the base- $m$  logarithm of both sides yields

$$\log_m \left( \frac{E_{n+1}}{E_n} \right) \sim -\gamma, \quad \text{or equivalently } \gamma \sim \log_m \left( \frac{E_n}{E_{n+1}} \right),$$

which provides us with the following:

$$\gamma_n = \log_m \left( \frac{E_n}{E_{n+1}} \right),$$

as a means of generating a sequence of approximations  $\{\gamma_k\}_{k=1}^\infty$ , which in theory should converge to  $\gamma$ . We note that the approximations  $\gamma_k$  should correspond to the slope of the line segments in the log-log convergence charts, as above.

In the experiments from which we collected our data, we halved the mesh size in each step and hence  $m = 2$ . The approximations obtained for the order  $\gamma$  can be found in the final columns of the tables in Appendix A. Examining those values

more closely, we can see that most of them lie fairly close to 1. Furthermore, they appear generally to be getting closer to 1, as the mesh is refined, with the approximations associated with the most refined mesh pairings having a mean value of 1.0301, across all configurations. This would suggest that our numerical scheme has order  $\gamma \approx 1$ , with the error in the approximations being  $\mathcal{O}(h)$ .

## 7.5 Convergence as $R \rightarrow \infty$

We now turn our attention to the truncation parameter  $R$ , seeking to empirically corroborate the assertion of Chapter 6, that the truncated solutions converge to the full solution as  $R \rightarrow \infty$ . As in the previous section we shall measure the convergence with respect to the norm on  $L_1([0, T], X_D) \times L_1([0, T], X_C)$ , as given in (7.14). Let  $u^R = (\underline{u}_D^R(t), u_C^R(x, t))$  denote our solution based on the interval truncated at  $R$  and  $u = (\underline{u}_D(t), u_C(x, t))$  the full solution over the semi-infinite domain. Then recalling Remark 6.2.7 and the bound given therein, the truncation error can be bounded like so:

$$\|u^R - u\| \leq (1 + k_c T) \int_0^T \|u_C^R(\cdot, s) - u_C(\cdot, s)\|_{X_C} ds,$$

where  $k_c$  is a constant, dependent on the functional  $c$  defined in Theorem 3.2.2. If we consider the form of the exact solution (7.9), then we see that the right-hand side above may be bounded by the integral of

$$\begin{aligned} |u_C^R(x, t) - u_C(x, t)| &\leq \chi_{(R, \infty)}(x) c_0(x) \\ &+ 2T \int_R^\infty y^{\alpha-\nu-1} c_0(y) |{}_1F_1(1-m, 2, t(x^\alpha - y^\alpha))| dy. \end{aligned} \quad (7.16)$$

Hence, aside from  $N$  and  $T$  and most obviously  $R$ , the error could potentially depend on the parameters  $\alpha$  and  $\nu$  as well as the initial distribution  $c_0$ . Further yet, the manner in which the right-hand side of (7.16) decays as  $R \rightarrow \infty$  provides some indication of the rate of convergence we might expect to observe.

However, returning to the matter at hand, the very reason for introducing the truncation was the difficulty in computationally representing the semi-infinite domain of our equation. A problem now re-encountered in trying to represent the full solution  $u$  in our error calculations. To counter this, we use a truncated solution  $u^{R_\infty} = (\underline{u}_D^{R_\infty}(t), u_C^{R_\infty}(x, t))$ , based on an interval up to some finite but large  $R_\infty$ , as a stand-in for the full solution  $u$ . We then consider the relative error between  $u^R$  and  $u^{R_\infty}$  as  $R \rightarrow R_\infty$ . As before, this is measured with respect to the  $L_1([0, T], X_D) \times L_1([0, T], X_C)$  norm, giving us

$$Error(u^R | u^{R_\infty}) = \frac{\|u^R - u^{R_\infty}\|}{\|u^{R_\infty}\|}, \quad (7.17)$$

where the norm  $\|\cdot\|$ , is the  $L_1([0, T], X_D) \times L_1([0, T], X_C)$  norm, as given in (7.14).

In order to confirm the convergence as  $R \rightarrow R_\infty$  and investigate the impact of the parameters identified as potentially significant, we conducted a series of numerical experiments over a range of model configurations. For the parameter settings, we considered all possible combinations of  $\alpha \in \{-1, 0, 0.5\}$  and  $\nu \in \{-1, 0\}$ , with  $N$  set at both 5 and 25. For each trial we set  $R_\infty = 100$  and considered a range of values for  $R$  between  $N$  and  $R_\infty$ . As a starting point, the initial mass distribution was taken to be constant:

$$d_{0i} = b, \text{ for } i = 1, \dots, N \quad \text{and} \quad c_0(x) = b, \text{ for } N < x < R_\infty,$$

with the value  $b$  selected to produce a total system mass of 100. The final time  $T$  was chosen in each case so as to allow the system, truncated at  $R_\infty$ , to reach a state near equilibrium. Owing to the significantly reduced computational time required by `numfrag.m` over `exactfrag.m`, we utilised fine-meshed numerical approximations of the solutions  $u^R$  and  $u^{R_\infty}$ , in place of exact solutions. The relative errors, as given by (7.17), were then evaluated using the Matlab code `truncerror.m`, which employs the rectangle rule to approximate the required integrals. For illustration purposes we have included the results for  $N = 5$ ,  $\alpha = 0.5$  and  $\nu = 0$  below. However, the full results obtained for all configurations may be found in Appendix A under the section for a uniform initial distribution.

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = 0.5$ , $\nu = 0$ , $T = 7$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$

Table 7.2: Experimental results for the case  $\alpha = 0.5$  and  $\nu = 0$  with a uniform initial distribution.

From an examination of the data, it is immediately apparent that the errors are converging towards zero as we let  $R \rightarrow R_\infty$ . However, a more detailed examination across the configurations, reveals some rather interesting relationships. Comparing dataset pairings, whereby only one factor is varied at a time, we can see that the parameter  $N$  has very little impact on the truncation error, whilst the parameters  $\alpha$  and  $\nu$  have almost no effect, certainly to the level of accuracy reported here. Considering the magnitude of the errors, for smaller values of  $R$  they appear to

be rather considerable, with a slow rate of convergence as  $R$  increases. It is only as  $R$  approaches  $R_\infty$ , that the errors reach a level which might be considered acceptable. Furthermore, as  $R$  is increased, the rate of convergence increases with it. This is perhaps to be expected from the profile of the initial mass distribution. The uniform profile means that particles of all sizes are equally common in the initial state. However, since larger particles carry more mass, each increase in  $R$  introduces a greater amount of mass than the previous one. Therefore, the proportion of the total mass associated with  $u^{R_\infty}$ , accounted for in  $u^R$ , grows at an increasing rate as  $R \rightarrow R_\infty$ .

In the previous experiments we imposed a uniform initial mass distribution which was constant up to the truncation point. However, if we consider the full equation with its unbounded domain, then the uniform distribution would violate the requirement for  $c_0$  to be  $L_1((N, \infty), x dx)$ , unless at some point it was indeed truncated. That being the case, we could simply take  $R$  to be greater than or equal to the truncation point and obtain the full solution. Therefore, for these next experiments we shall employ an initial mass distribution featuring a negative exponential profile. Such a profile not only allows for infinite support whilst having finite mass, but would also appear to offer a realistic fit to the previously observed solutions, which are driven by the  $e^{-x^\alpha t}$  factor featuring in equation (7.9). Hence, we shall assume an initial state of the form

$$d_{0i} = be^{ci}, \text{ for } i = 1, \dots, N \quad \text{and} \quad c_0(x) = be^{cx}, \text{ for } x > N, \quad (7.18)$$

where  $b > 0$  and  $c < 0$  are constants to be selected. The Matlab code `Init_fit.m`, contained in Appendix B, computes these values for us, subject to the following criteria. When provided with an  $N$ ,  $R$  and a proportion  $p$ , the code computes the value of  $c$ , such that if the initial state (7.18) were truncated at  $R$ , the mass associated with the truncated initial state would account for a proportion  $p$  of the mass of the untruncated distribution. It does this using a bisection approach, with the answer provided having an accuracy within a user-specified tolerance. The value of  $b$  is then selected so that the  $R_\infty$  truncated distribution has an associated total mass of  $TM$ , which again is specified by the user.

Once again we conducted a range of numerical experiments using the numerical solution code `numfrag.m`. The same parameter values of  $\alpha \in \{-1, 0, 0.5\}$ ,  $\nu \in \{-1, 0\}$ ,  $N \in \{5, 25\}$  and  $R_\infty = 100$  were utilised. Given these choices of  $N$  and  $R_\infty$ , we made use of the program `Init_fit.m` to fit our initial mass distribution so that the  $R_\infty$  truncation accounted for a proportion 0.99 of the mass of the untruncated case. The value of  $b$  was then chosen to give a total truncated mass of 100. For  $N = 5$ , this resulted in the choices  $b = 4.4088 \times 10^{-1}$  and  $c = -6.6320 \times 10^{-2}$ , whilst  $N = 25$  gave us  $b = 4.3985 \times 10^{-1}$  and  $c = -6.6320 \times 10^{-2}$ . The results obtained for the case  $N = 5$ ,  $\alpha = 0.5$  and  $\nu = 0$  are included below, allowing a ready comparison with those of Table 7.2. For the full set of numerical results from

all experimental configurations the reader is directed towards Appendix A, where they appear under the section for the negative exponential initial distribution.

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0.5$ , $\nu = 0$ , $T = 7$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Table 7.3: Experimental results for the case  $\alpha = 0.5$  and  $\nu = 0$  with a negative exponential initial distribution.

Examining the data from the experiments, we can see that as before the error appears to converge towards zero as  $R \rightarrow R_\infty$ . Once again, comparing between configurations reveals that the parameters  $N$ ,  $\alpha$  and  $\nu$  seem to have little effect on the truncation error. Comparing the results between the uniform and negative exponential cases, we can see that the truncation errors for the negative exponential are less than those for corresponding uniform distribution, and that the rate of convergence is faster. This is perhaps to be expected, as in contrast to the uniform initial state, with the negative exponential the bulk of the mass is accounted for by the smaller particles.

To summarise our experimental findings, the error introduced by truncating the domain at  $R$  appears to converge to zero as  $R$  is increased. Furthermore, the experiments suggest that this error is independent of the model parameters  $N$ ,  $\alpha$  and  $\nu$ , depending largely on the truncation point  $R$  and the initial mass profile, with the rate of convergence being determined by the initial mass profile.

In this chapter we conducted a range of numerical experiments in order to test the findings of the previous chapters and hopefully gain further insight. To begin with, we considered a degenerate case of the purely continuous model, plotting its solution and considering the associated mass through time. We found that, as predicted in the literature, the solution experienced a loss of total mass. As a response to this, we examined the (numerical) solutions to an analogous form of our new model and found that, in contrast, it conserved mass. Following this, we varied the model parameters and observed the effect on the solution. We found the behaviour exhibited was as one would expect from the physical interpretation of the model and its parameters. Given the choices of Section 7.2, we were able to derive an exact solution for the class of model under consideration. Therefore

we proceeded to examine the accuracy of the numerical solutions. Conducting a range of experiments with varying model parameter choices and mesh refinements, we experimentally established that the error in our numerical solutions was  $\mathcal{O}(h)$ , where  $h$  was the maximum interval length for the mass-variable and  $k_1 h < \Delta t < k_2 h$ . Finally, we examined the error induced by the truncation of the domain of the equation, when we form our numerical solutions. The scale of this error was found to depend largely on the point  $R$  at which the interval was truncated and the profile of the initial mass distribution: the larger the value of  $R$  and the faster the decay of the distribution, the smaller the error.

# Chapter 8

## Summary and Future Areas of Research

In this final chapter we present a summary of the material from the thesis and outline the contributions made. The chapter is completed with a section indicating possible areas for future research.

### 8.1 Summary of Work Completed

The main results covered in this thesis concern the development and analysis of a mixed discrete–continuous fragmentation model. The impetus for the development of such a model was the inherent ‘shattering’ problem which can arise with a purely continuous model when the fragmentation rate blows up as the particle mass goes to zero, as discussed in Section 1.4 and observed in Section 7.1. This problem was previously addressed in [38] by the introduction of a cut-off, such that if particles have mass below this then they are unable to fragment. We feel that our mixed model offers a more elegant solution, which more closely reflects the true nature of such processes and given the similarities between the discrete and continuous models it seems natural to combine them in this way.

In Chapter 3, we began by introducing our new hybrid discrete–continuous fragmentation model, which took the form of an integro–differential equation coupled with a system of ordinary differential equations. As far as we are aware, this represents the first instance of such a hybrid model in the area of coagulation–fragmentation models. Recasting these equations in the setting of the appropriate Banach spaces, and using the theory of semigroups, in particular the Kato–Voigt perturbation theorem and material on operator matrices, we were able to establish, under standard restrictions on the model, the existence of a unique strong solution to our system of equations. From the existence of this strong solution, we were able to deduce the existence of a unique classical solution to our original model. Further, the solution was shown to preserve non-negativity and conserve mass,

two necessary attributes considering the physical nature of the problem, especially given the motivation for the development of the new model to counter shattering mass loss.

Given that most of the existing models in the field do not yield closed-form solutions, and require numerical methods for their approximate solution, it is reasonable to believe that this could be the case for many examples of our new class of model. Therefore, in Chapter 4 we developed a numerical scheme for the approximate solution of a truncated version of our model, whereby the continuous mass interval was truncated at an upper limit, which we denoted by  $R$ . As with the analytically ‘obtained’ solutions of the previous chapter, the approximate solutions were shown to preserve non-negativity and conserve mass, provided certain restrictions on the mesh were satisfied.

In Chapter 5, using a common weak compactness argument, we were able to prove the existence of a subsequence of our family of approximations, that is weakly convergent to a weak solution of our truncated set of equations. In much of the literature on the numerical approximation of coagulation–fragmentation equations, this is the extent of the results provided. However, there are many unanswered questions, such as:

1. Could the scheme converge to multiple solutions (different subsequences resulting in different solutions)?
2. How regular are the solutions, are they differentiable and how do they relate to those obtained in Chapter 3?
3. What happens as we let the truncation parameter  $R \rightarrow \infty$ ?

In Chapter 6, by relating the material on strong semigroup solutions from Chapter 3, to the truncated weak solutions of Chapter 5, we were able to resolve these issues. First to begin with, we were able to demonstrate that the solutions obtained as limits of our numerical approximations must necessarily be unique, and therefore they must be differentiable classical solutions to the truncated versions of our equations. This result exceeds those found in the literature, which typically offer only weak solutions with generally no guarantee of uniqueness. The theoretical study was completed by examining the truncated solutions as we let  $R \rightarrow \infty$ , confirming that in the limit we obtain the full strong solution, as asserted in Chapter 3.

The project was completed with a numerical experimental study, as detailed in Chapter 7, where we examined the behaviour of a number of different cases for the hybrid fragmentation model. In each example, the numerical solutions behaved as predicted, remaining non-negative and conserving mass. We were also able to experimentally confirm the convergence of our numerical scheme to the exact solutions.

## 8.2 Areas for Future Work and Research

### 8.2.1 A Mixed Discrete–Continuous Coagulation–Fragmentation Model

Having considered a model involving only fragmentation in this work, one area for possible examination is the introduction of a reverse coagulation process, whereby pairs of particles can join to form a larger particle. In the literature these processes are often considered together, and therefore this would seem an obvious addition to the model. Here we shall briefly consider the additional terms required for the introduction of such a process to our model, before indicating a possible approach to the analysis of the resulting equations.

#### 8.2.1.1 Additional Modelling Terms

As before, let  $u_D$  and  $u_C$  denote the particle mass density within the discrete and continuous regimes, respectively. We introduce the function  $k(x, y)$ , which is the continuous coagulation kernel giving the rate at which continuous mass particles with masses  $x$  and  $y$  join together. Also, we define the values  $k_{i,j}$  to give the rate at which discrete mass  $i$ -mers and  $j$ -mers combine. Finally the functions  $k_i(y)$  provide the rate at which a discrete mass  $i$ -mer joins with a continuous mass particle of mass  $y > N$ . The physical nature of the process demands that each of  $k(x, y)$ ,  $k_{i,j}$  and  $k_i(y)$  be non-negative, with  $k(x, y)$  and  $k_{i,j}$  symmetric.

Considering the effect of coagulation on the continuous mass regime, the associated change in the density  $u_C(x, t)$  is modelled by the expression

$$\begin{aligned}
 (N_C(u_D, u_C))(x, t) = & -u_C(x, t) \left\{ \sum_{j=1}^N k_j(x) u_{Dj}(t) + \int_N^\infty k(x, y) u_C(y, t) dy \right\} \\
 & + \frac{\chi_I(x)}{2} \left\{ 2 \sum_{j=1}^{\lceil x \rceil - N - 1} k_j(x - j) u_{Dj}(t) u_C(x - j, t) + \chi_N(x) \sum_{j=x-N}^N k_{j, x-j} u_{Dj}(t) u_{D(x-j)}(t) \right\} \\
 & + \frac{\chi_J(x)}{2} \left\{ 2 \sum_{j=1}^N k_j(x - j) u_{Dj}(t) u_C(x - j, t) + \int_N^{x-N} k(y, x - y) u_C(y, t) u_C(x - y, t) dy \right\},
 \end{aligned} \tag{8.1}$$

where  $I = (N, 2N]$  and  $J = (2N, \infty)$ . The first two terms appearing on the right are loss terms and account for the loss of particles of mass  $x$ , which arises when such a particle joins with some other particle. The terms involving the characteristic equations are gain terms and account for the increase in particles of mass  $x$  due to the joining together of two suitably sized smaller particles. If we consider the case of  $x \in I$ , then we see that at least one of the contributing particles must

be from the discrete mass regime, although if  $x$  is not an integer value then one of the constituent particles must be from the continuous mass regime. Whereas when  $x \in J$ , we must have at least one of the contributing particles coming from the continuous mass regime. The requirement for multiple gain terms arises as we must consider all combinations of particle types which could possibly give rise to a particle of mass  $x$ .

The change in the continuous mass regime density is then governed by the following equation:

$$\begin{aligned} \frac{\partial u_C(x, t)}{\partial t} &= (\mathcal{F}_C u_C)(x, t) + (N_C(u_D, u_C))(x, t), \quad x > N, t > 0, \\ u_C(x, 0) &= c_0(x), \end{aligned} \quad (8.2)$$

where  $\mathcal{F}_C u_C$  is the continuous regime fragmentation term, which is given by the right-hand side of continuous regime fragmentation equation (3.1).

If we now consider the discrete mass regime, then the change in the concentration of  $i$ -mers due to coagulation is given by

$$\begin{aligned} (N_D(u_D, u_C)(t))_i &= -u_{Di}(t) \left\{ \sum_{j=1}^N k_{i,j} u_{Dj}(t) + \int_N^\infty k_i(y) u_C(y, t) dy \right\} \\ &\quad + \frac{1}{2} \sum_{j=1}^{i-1} k_{j,i-j} u_{Dj}(t) u_{D(i-j)}(t). \end{aligned} \quad (8.3)$$

As before, the first two terms are loss terms accounting for the loss of  $i$ -mers when any such particle joins some other particle. The last term is a gain term. In contrast to the continuous regime, we only require a single gain term as clearly both contributing particles must come from the discrete mass regime.

The change in the particle density  $u_D$  of the discrete regime is then described by the equation below:

$$\begin{aligned} \frac{du_{Di}(t)}{dt} &= \mathcal{F}_D(u_D, u_F)_i + (N_D(u_D, u_C)(t))_i, \quad i = 1, \dots, N, \quad t > 0, \\ u_D(0) &= d_0, \end{aligned} \quad (8.4)$$

where the fragmentation term  $\mathcal{F}_D(u_D, u_F)_i$  is provided by the right-hand side of the discrete mass regime fragmentation equation (3.2).

### 8.2.1.2 Potential Approach for the Analysis

The usual approach when using semigroup theory to prove the existence of solutions for such combined coagulation–fragmentation equations is to formulate them as a semilinear abstract Cauchy problem. In this case, the additional coagulation terms  $N_D$  and  $N_C$  are combined and treated as a nonlinear perturbation operator  $\mathcal{N}$ , acting on the appropriate product space. The task is then to show that the operator  $\mathcal{N}$ , possesses certain properties, namely that it satisfies a local Lipschitz condition and is Fréchet differentiable with continuous derivative. Doing so allows us to establish the existence of a unique, local in time, strong solution to the semilinear ACP, [14, Theorems 3.22, 3.30 and 3.32].

Commonly a change of spaces is made before carrying out this analysis, with the usual choice being a space of the form  $L_1(\mathbb{I}, (1+x) dx)$ , where  $\mathbb{I}$  is the appropriate interval domain, or if considering a discrete model the analogous weighted  $l_1$  space. This is done for mathematical convenience, as the new norm more easily allows us to establish the properties described above. However in our case, as our interval  $(N, \infty)$  is away from zero, such a space would be equivalent to our  $X_C$  from Chapter 3 and since  $X_D$  is finite-dimensional all norms are automatically equivalent. That being said, one may wish to give some further consideration to the space in which to work as the term involving  $\chi_N$  in  $N_C$  will vanish if working in  $X_C$ .

It is then common to show that the solution remains positive on its maximal interval of existence and that it does not produce a finite time blow-up and hence is a global in time strong solution [68, Chapter 6, Theorem 1.4]. Such an approach was adopted in the works of [46, 12, 56], amongst others.

## 8.2.2 Variation of the Transition Parameter $N$

The introduction of the mass cut-off parameter  $N$  raises the question of how the value of  $N$  should be selected. It would be of interest to examine numerically how varying  $N$  affects the results we obtain and the computational run-times for the numerical method. Ideally, it would be advantageous to establish criteria for the selection of an optimum  $N$  given the modelling choices. Taking this idea of the choice of  $N$  further, we might consider a family of hybrid models, parameterised by the cut-off  $N$ , and we might wonder whether, as  $N \rightarrow \infty$ , we obtain the solutions for a corresponding fully discrete equation. A further possibility relating to the parameter  $N$ , which we might consider, is whether it would be possible to introduce a cut-off  $N(t)$ , which has a time dependence, allowing for an adaptive change as the system evolves. This might be especially useful in the case of a nonautonomous model, with time-dependent fragmentation coefficients  $a$  and  $b$ , as was considered in [5], for the purely continuous case.

### 8.2.3 Further Example Models and Applications

In Chapter 7 we introduced a particular form of our hybrid model and investigated the behaviour of the resulting solutions. However, as was shown in Table 1.1, and can be found in [10, Section 8.2], there exist a number of forms and kernel choices for the standard continuous and discrete coagulation–fragmentation models. Therefore, one area where we might expect further work to be advantageous is in the development of further hybrid models, allowing for the modelling of a wider range of physical scenarios. The standard continuous models appear to provide candidates for the continuous equation (3.1). However, given a  $b(x|y)$ , we must find a corresponding set of  $b_i(y)$  functions which satisfy (3.3) and select suitable rates for our discrete equation (3.2).

An area of further study which we would be keen to see, involves the application of hybrid models, of the type introduced here, to concrete practical problems. In a number of practical application areas, a distinction is made between the behaviour of particles on different length scales, for example between ‘dust and boulders’ in rock crushing [76]. In cases like these, the application of a hybrid model may provide a suitable framework to accommodate these differences and provide a better modelling solution. It seems clear that these last two areas go hand in hand, with the development of a catalogue of hybrid models leading to a greater possibility of the useful application of such a model. Such an application would be highly satisfying and provides further justification for the ideas and theory developed within this thesis.

# Appendix

## A - Experimental Numerical Data

The following tables detail the experiments completed in connection with the experiments of Chapter 7. Each table provides the parameter values for the model setup, the mesh parameters for each of the approximation runs and the associated relative errors. The data contained within the tables are reported to an accuracy of 5 significant figures. However, wherever these quantities have been utilised in any computations or calculations, it is the underlying values (accurate to 16 significant figures) that have been used.

### Data for Section 7.4.2

Parameters: $N = 5, R = 15, T = 6, \alpha = 0.5, \nu = 0,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 5.8594 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	0.62500	0.18750	$6.9714 \times 10^{-2}$	NA
2	0.31250	$9.3750 \times 10^{-2}$	$3.2251 \times 10^{-2}$	1.1121
3	0.15625	$4.6875 \times 10^{-2}$	$1.5508 \times 10^{-2}$	1.0563
4	$7.8125 \times 10^{-2}$	$2.3438 \times 10^{-2}$	$7.5624 \times 10^{-3}$	1.0361
5	$3.9063 \times 10^{-2}$	$1.1719 \times 10^{-2}$	$3.7215 \times 10^{-3}$	1.0229

Parameters: $N = 5, R = 15, T = 6, \alpha = 0.5, \nu = -0.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 5.8594 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	0.62500	0.18750	$6.5675 \times 10^{-2}$	NA
2	0.31250	$9.3750 \times 10^{-2}$	$3.0250 \times 10^{-2}$	1.1184
3	0.15625	$4.6875 \times 10^{-2}$	$1.4522 \times 10^{-2}$	1.0587
4	$7.8125 \times 10^{-2}$	$2.3438 \times 10^{-2}$	$7.0778 \times 10^{-3}$	1.0369
5	$3.9063 \times 10^{-2}$	$1.1719 \times 10^{-2}$	$3.4888 \times 10^{-3}$	1.0206

Parameters: $N = 5, R = 15, T = 6, \alpha = 0.5, \nu = -1,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 5.8594 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	0.62500	0.18750	$5.8886 \times 10^{-2}$	NA
2	0.31250	$9.3750 \times 10^{-2}$	$2.7008 \times 10^{-2}$	1.1245
3	0.15625	$4.6875 \times 10^{-2}$	$1.2945 \times 10^{-2}$	1.0610
4	$7.8125 \times 10^{-2}$	$2.3438 \times 10^{-2}$	$6.3049 \times 10^{-3}$	1.0379
5	$3.9063 \times 10^{-2}$	$1.1719 \times 10^{-2}$	$3.1145 \times 10^{-3}$	1.0175

Parameters: $N = 5, R = 15, T = 6, \alpha = 0.5, \nu = -1.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 5.8594 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	0.62500	0.18750	$4.7407 \times 10^{-2}$	NA
2	0.31250	$9.3750 \times 10^{-2}$	$2.1672 \times 10^{-2}$	1.1293
3	0.15625	$4.6875 \times 10^{-2}$	$1.0392 \times 10^{-2}$	1.0604
4	$7.8125 \times 10^{-2}$	$2.3438 \times 10^{-2}$	$5.0771 \times 10^{-3}$	1.0333
5	$3.9063 \times 10^{-2}$	$1.1719 \times 10^{-2}$	$2.5447 \times 10^{-3}$	$9.9653 \times 10^{-1}$

Parameters: $N = 5, R = 15, T = 10, \alpha = 0.1, \nu = 0,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 9.7656 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	0.62500	$1.2961 \times 10^{-1}$	NA
2	0.62500	0.31250	$5.7604 \times 10^{-2}$	1.1700
3	0.31250	0.15625	$2.7323 \times 10^{-2}$	1.0760
4	0.15625	$7.8125 \times 10^{-2}$	$1.3264 \times 10^{-2}$	1.0426
5	$7.8125 \times 10^{-2}$	$3.9063 \times 10^{-2}$	$6.4870 \times 10^{-3}$	1.0319
6	$3.9063 \times 10^{-2}$	$1.9531 \times 10^{-2}$	$3.1879 \times 10^{-3}$	1.0249

Parameters: $N = 5, R = 15, T = 10, \alpha = 0.1, \nu = -0.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 9.7656 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	0.62500	$1.2636 \times 10^{-1}$	NA
2	0.62500	0.31250	$5.5508 \times 10^{-2}$	1.1868
3	0.31250	0.15625	$2.6222 \times 10^{-2}$	1.0820
4	0.15625	$7.8125 \times 10^{-2}$	$1.2707 \times 10^{-2}$	1.0451
5	$7.8125 \times 10^{-2}$	$3.9063 \times 10^{-2}$	$6.2133 \times 10^{-3}$	1.0322
6	$3.9063 \times 10^{-2}$	$1.9531 \times 10^{-2}$	$3.0620 \times 10^{-3}$	1.0209

Parameters: $N = 5, R = 15, T = 10, \alpha = 0.1, \nu = -1,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 9.7656 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	0.62500	$1.1765 \times 10^{-1}$	NA
2	0.62500	0.31250	$5.1181 \times 10^{-2}$	1.2008
3	0.31250	0.15625	$2.4091 \times 10^{-2}$	1.0871
4	0.15625	$7.8125 \times 10^{-2}$	$1.1656 \times 10^{-2}$	1.0474
5	$7.8125 \times 10^{-2}$	$3.9063 \times 10^{-2}$	$5.6962 \times 10^{-3}$	1.0330
6	$3.9063 \times 10^{-2}$	$1.9531 \times 10^{-2}$	$2.8142 \times 10^{-3}$	1.0173

Parameters: $N = 5, R = 15, T = 10, \alpha = 0.1, \nu = -1.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 9.7656 \times 10^{-3}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	0.62500	$9.9180 \times 10^{-2}$	NA
2	0.62500	0.31250	$4.2822 \times 10^{-2}$	1.2117
3	0.31250	0.15625	$2.0135 \times 10^{-2}$	1.0886
4	0.15625	$7.8125 \times 10^{-2}$	$9.7413 \times 10^{-3}$	1.0475
5	$7.8125 \times 10^{-2}$	$3.9063 \times 10^{-2}$	$4.7700 \times 10^{-3}$	1.0301
6	$3.9063 \times 10^{-2}$	$1.9531 \times 10^{-2}$	$2.3794 \times 10^{-3}$	1.0034

Parameters: $N = 5, R = 15, T = 35, \alpha = -0.5, \nu = 0,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 3.4180 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	2.1875	$9.9023 \times 10^{-2}$	NA
2	0.62500	1.0938	$4.4984 \times 10^{-2}$	1.1383
3	0.31250	$5.4688 \times 10^{-1}$	$2.1511 \times 10^{-2}$	1.0643
4	0.15625	$2.7344 \times 10^{-1}$	$1.0482 \times 10^{-2}$	1.0371
5	$7.8125 \times 10^{-2}$	$1.3672 \times 10^{-1}$	$5.1390 \times 10^{-3}$	1.0284
6	$3.9063 \times 10^{-2}$	$6.8359 \times 10^{-2}$	$2.5390 \times 10^{-3}$	1.0172

Parameters: $N = 5, R = 15, T = 35, \alpha = -0.5, \nu = -0.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 3.4180 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	2.1875	$9.8691 \times 10^{-2}$	NA
2	0.62500	1.0938	$4.4051 \times 10^{-2}$	1.1637
3	0.31250	$5.4688 \times 10^{-1}$	$2.0944 \times 10^{-2}$	1.0726
4	0.15625	$2.7344 \times 10^{-1}$	$1.0181 \times 10^{-2}$	1.0407
5	$7.8125 \times 10^{-2}$	$1.3672 \times 10^{-1}$	$4.9896 \times 10^{-3}$	1.0288
6	$3.9063 \times 10^{-2}$	$6.8359 \times 10^{-2}$	$2.4727 \times 10^{-3}$	1.0129

Parameters: $N = 5, R = 15, T = 35, \alpha = -0.5, \nu = -1,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 3.4180 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	2.1875	$9.5962 \times 10^{-2}$	NA
2	0.62500	1.0938	$4.1989 \times 10^{-2}$	1.1925
3	0.31250	$5.4688 \times 10^{-1}$	$1.9828 \times 10^{-2}$	1.0824
4	0.15625	$2.7344 \times 10^{-1}$	$9.6127 \times 10^{-3}$	1.0446
5	$7.8125 \times 10^{-2}$	$1.3672 \times 10^{-1}$	$4.7077 \times 10^{-3}$	1.0299
6	$3.9063 \times 10^{-2}$	$6.8359 \times 10^{-2}$	$2.3390 \times 10^{-3}$	1.0091

Parameters: $N = 5, R = 15, T = 25, \alpha = -0.5, \nu = -1.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 2.4414 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	1.5625	$7.9232 \times 10^{-2}$	NA
2	0.62500	$7.8125 \times 10^{-1}$	$3.5779 \times 10^{-2}$	1.1470
3	0.31250	$3.9063 \times 10^{-1}$	$1.7096 \times 10^{-2}$	1.0654
4	0.15625	$1.9531 \times 10^{-1}$	$8.3247 \times 10^{-3}$	1.0382
5	$7.8125 \times 10^{-2}$	$9.7656 \times 10^{-2}$	$4.0853 \times 10^{-3}$	1.0270
6	$3.9063 \times 10^{-2}$	$4.8828 \times 10^{-2}$	$2.0396 \times 10^{-3}$	1.0021

Parameters: $N = 5, R = 15, T = 100, \alpha = -1, \nu = 0,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 4.8828 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	3.1250	$1.7834 \times 10^{-2}$	NA
2	0.62500	1.5625	$8.7590 \times 10^{-3}$	1.0258
3	0.31250	$7.8125 \times 10^{-1}$	$4.3325 \times 10^{-3}$	1.0155
4	0.15625	$3.9063 \times 10^{-1}$	$2.1432 \times 10^{-3}$	1.0155
5	$7.8125 \times 10^{-2}$	$1.9531 \times 10^{-1}$	$1.0574 \times 10^{-3}$	1.0192
6	$3.9063 \times 10^{-2}$	$9.7656 \times 10^{-2}$	$5.2312 \times 10^{-4}$	1.0153

Parameters: $N = 5, R = 15, T = 100, \alpha = -1, \nu = -0.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 4.8828 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	3.1250	$3.5512 \times 10^{-2}$	NA
2	0.62500	1.5625	$1.7144 \times 10^{-2}$	1.0506
3	0.31250	$7.8125 \times 10^{-1}$	$8.4218 \times 10^{-3}$	1.0255
4	0.15625	$3.9063 \times 10^{-1}$	$4.1546 \times 10^{-3}$	1.0194
5	$7.8125 \times 10^{-2}$	$1.9531 \times 10^{-1}$	$2.0511 \times 10^{-3}$	1.0183
6	$3.9063 \times 10^{-2}$	$9.7656 \times 10^{-2}$	$1.0227 \times 10^{-3}$	1.0039

Parameters: $N = 5, R = 15, T = 100, \alpha = -1, \nu = -1,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 4.8828 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	3.1250	$3.4859 \times 10^{-2}$	NA
2	0.62500	1.5625	$1.6566 \times 10^{-2}$	1.0733
3	0.31250	$7.8125 \times 10^{-1}$	$8.0831 \times 10^{-3}$	1.0353
4	0.15625	$3.9063 \times 10^{-1}$	$3.9772 \times 10^{-3}$	1.0232
5	$7.8125 \times 10^{-2}$	$1.9531 \times 10^{-1}$	$1.9643 \times 10^{-3}$	1.0177
6	$3.9063 \times 10^{-2}$	$9.7656 \times 10^{-2}$	$9.8610 \times 10^{-4}$	$9.9421 \times 10^{-1}$

Parameters: $N = 5, R = 15, T = 100, \alpha = -1, \nu = -1.5,$ $h_{exact} = 1.9531 \times 10^{-2}, \Delta t_{exact} = 4.8828 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	3.1250	$3.3176 \times 10^{-2}$	NA
2	0.62500	1.5625	$1.5562 \times 10^{-2}$	1.0922
3	0.31250	$7.8125 \times 10^{-1}$	$7.5523 \times 10^{-3}$	1.0430
4	0.15625	$3.9063 \times 10^{-1}$	$3.7082 \times 10^{-3}$	1.0262
5	$7.8125 \times 10^{-2}$	$1.9531 \times 10^{-1}$	$1.8324 \times 10^{-3}$	1.0170
6	$3.9063 \times 10^{-2}$	$9.7656 \times 10^{-2}$	$9.2595 \times 10^{-4}$	$9.8473 \times 10^{-1}$

*Remark.* In the computation of the exact solution, when a larger final time  $T$  is used, we can encounter issues with blow-up in the computed values. The source of these problems lies with the larger values which occur in the calculation of the matrix exponential  $e^{-sC}$  from (7.12), when  $s$  must range up to such a  $T$ . When these large values are multiplied with other computed values, any errors present are scaled up significantly. This becomes an issue when we consider larger, negative values of the parameter  $\alpha$ . Such values of  $\alpha$  result in a relatively low average fragmentation rate, and as a result the time required for the system to reach a near equilibrium state is extended. In particular, the choice of  $\alpha = -2$  resulted in a runtime to equilibrium which was beyond the point where blow-up was encountered. For the case  $\alpha = -2$ , in order to assess the convergence of our approximations over a time period up to equilibrium, we resorted to the use of a fine-meshed numerical solution as a substitute for the exact solution. The data corresponding to these examples can be found below.

Parameters: $N = 5, R = 15, T = 1000, \alpha = -2, \nu = -0,$ $h_{exact} = 9.7656 \times 10^{-3}, \Delta t_{exact} = 6.1035 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	7.8125	$6.3318 \times 10^{-3}$	NA
2	0.62500	3.9062	$3.0082 \times 10^{-3}$	1.0737
3	0.31250	1.9531	$1.5023 \times 10^{-3}$	1.0017
4	0.15625	$9.7656 \times 10^{-1}$	$7.3949 \times 10^{-4}$	1.0225
5	$7.8125 \times 10^{-2}$	$4.8828 \times 10^{-1}$	$3.5517 \times 10^{-4}$	1.0580
6	$3.9063 \times 10^{-2}$	$2.4414 \times 10^{-1}$	$1.6235 \times 10^{-4}$	1.1294

Parameters: $N = 5, R = 15, T = 1000, \alpha = -2, \nu = -0.5,$ $h_{exact} = 9.7656 \times 10^{-3}, \Delta t_{exact} = 6.1035 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	7.8125	$6.9894 \times 10^{-3}$	NA
2	0.62500	3.9062	$3.3089 \times 10^{-3}$	1.0788
3	0.31250	1.9531	$1.6254 \times 10^{-3}$	1.0256
4	0.15625	$9.7656 \times 10^{-1}$	$7.9438 \times 10^{-4}$	1.0329
5	$7.8125 \times 10^{-2}$	$4.8828 \times 10^{-1}$	$3.8143 \times 10^{-4}$	1.0584
6	$3.9063 \times 10^{-2}$	$2.4414 \times 10^{-1}$	$1.7528 \times 10^{-0}$	1.1218

Parameters: $N = 5, R = 15, T = 1000, \alpha = -2, \nu = -1,$ $h_{exact} = 9.7656 \times 10^{-3}, \Delta t_{exact} = 6.1035 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	7.8125	$8.0478 \times 10^{-3}$	NA
2	0.62500	3.9062	$3.8644 \times 10^{-3}$	1.0584
3	0.31250	1.9531	$1.8864 \times 10^{-3}$	1.0346
4	0.15625	$9.7656 \times 10^{-1}$	$9.2176 \times 10^{-4}$	1.0331
5	$7.8125 \times 10^{-2}$	$4.8828 \times 10^{-1}$	$4.4504 \times 10^{-4}$	1.0505
6	$3.9063 \times 10^{-2}$	$2.4414 \times 10^{-1}$	$2.0750 \times 10^{-4}$	1.1008

Parameters: $N = 5, R = 15, T = 1000, \alpha = -2, \nu = -1.5,$ $h_{exact} = 9.7656 \times 10^{-3}, \Delta t_{exact} = 6.1035 \times 10^{-2}$				
$n$	$h_n$	$\Delta t$	Relative Error $E_n$	$\gamma_{n-1}$
1	1.2500	7.8125	$9.4311 \times 10^{-3}$	NA
2	0.62500	3.9062	$4.4871 \times 10^{-3}$	1.0716
3	0.31250	1.9531	$2.1911 \times 10^{-3}$	1.0341
4	0.15625	$9.7656 \times 10^{-1}$	$1.0733 \times 10^{-3}$	1.0296
5	$7.8125 \times 10^{-2}$	$4.8828 \times 10^{-1}$	$5.2127 \times 10^{-4}$	1.0420
6	$3.9063 \times 10^{-2}$	$2.4414 \times 10^{-1}$	$2.4540 \times 10^{-4}$	1.0869

## Data for Section 7.5

### Uniform Initial Distribution

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = 0.5$ , $\nu = 0$ , $T = 7$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 1.9950 \times 10^{-2}$ , $c = 0$ , $\alpha = 0.5$ , $\nu = 0$ , $T = 7$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$9.0773 \times 10^{-1}$	$8.3790 \times 10^{-1}$	$7.4813 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3840 \times 10^{-1}$	$5.0873 \times 10^{-1}$	$3.5910 \times 10^{-1}$	$1.8953 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7257 \times 10^{-2}$	$5.8953 \times 10^{-2}$	$3.9501 \times 10^{-2}$	$1.9850 \times 10^{-2}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = 0.5$ , $\nu = -1$ , $T = 6$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 1.9950 \times 10^{-2}$ , $c = 0$ , $\alpha = 0.5$ , $\nu = -1$ , $T = 6$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$9.0773 \times 10^{-1}$	$8.3791 \times 10^{-1}$	$7.4813 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3840 \times 10^{-1}$	$5.0873 \times 10^{-1}$	$3.5910 \times 10^{-1}$	$1.8953 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7257 \times 10^{-2}$	$5.8953 \times 10^{-2}$	$3.9501 \times 10^{-2}$	$1.9850 \times 10^{-2}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = 0$ , $\nu = 0$ , $T = 20$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$
Parameters: $N = 25$ , $R_\infty = 100$ , $b = 1.9950 \times 10^{-2}$ , $c = 0$ , $\alpha = 0$ , $\nu = 0$ , $T = 20$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$9.0773 \times 10^{-1}$	$8.3791 \times 10^{-1}$	$7.4813 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3840 \times 10^{-1}$	$5.0873 \times 10^{-1}$	$3.5910 \times 10^{-1}$	$1.8953 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7257 \times 10^{-2}$	$5.8953 \times 10^{-2}$	$3.9501 \times 10^{-2}$	$1.9850 \times 10^{-2}$
Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = 0$ , $\nu = -1$ , $T = 15$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$
Parameters: $N = 25$ , $R_\infty = 100$ , $b = 1.9950 \times 10^{-2}$ , $c = 0$ , $\alpha = 0$ , $\nu = -1$ , $T = 15$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$9.0773 \times 10^{-1}$	$8.3791 \times 10^{-1}$	$7.4813 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3840 \times 10^{-1}$	$5.0873 \times 10^{-1}$	$3.5910 \times 10^{-1}$	$1.8953 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7257 \times 10^{-2}$	$5.8953 \times 10^{-2}$	$3.9501 \times 10^{-2}$	$1.9850 \times 10^{-2}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = -1$ , $\nu = 0$ , $T = 750$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 1.9950 \times 10^{-2}$ , $c = 0$ , $\alpha = -1$ , $\nu = 0$ , $T = 750$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	NA	$9.0773 \times 10^{-1}$	$8.3790 \times 10^{-1}$	$7.4813 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3840 \times 10^{-1}$	$5.0873 \times 10^{-1}$	$3.5910 \times 10^{-1}$	$1.8953 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7257 \times 10^{-2}$	$5.8953 \times 10^{-2}$	$3.9501 \times 10^{-2}$	$1.9850 \times 10^{-2}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 1.9990 \times 10^{-2}$ , $c = 0$ , $\alpha = -1$ , $\nu = -1$ , $T = 600$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	$9.7701 \times 10^{-1}$	$9.0955 \times 10^{-1}$	$8.3958 \times 10^{-1}$	$7.4963 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3968 \times 10^{-1}$	$5.0975 \times 10^{-1}$	$3.5982 \times 10^{-1}$	$1.8991 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7451 \times 10^{-2}$	$5.9070 \times 10^{-2}$	$3.9580 \times 10^{-2}$	$1.9890 \times 10^{-2}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 1.9950 \times 10^{-2}$ , $c = 0$ , $\alpha = -1$ , $\nu = -1$ , $T = 600$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	NA	$9.0773 \times 10^{-1}$	$8.3791 \times 10^{-1}$	$7.4813 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$6.3840 \times 10^{-1}$	$5.0873 \times 10^{-1}$	$3.5910 \times 10^{-1}$	$1.8953 \times 10^{-1}$
$R$	95	97	98	99
Relative Error	$9.7257 \times 10^{-2}$	$5.8953 \times 10^{-2}$	$3.9501 \times 10^{-2}$	$1.9850 \times 10^{-2}$

**Negative Exponential Initial Distribution**

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0.5$ , $\nu = 0$ , $T = 7$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 4.3985 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0.5$ , $\nu = 0$ , $T = 7$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$3.9877 \times 10^{-1}$	$2.4730 \times 10^{-1}$	$1.4661 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3059 \times 10^{-2}$	$4.4307 \times 10^{-2}$	$2.1244 \times 10^{-2}$	$7.7661 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3451 \times 10^{-3}$	$1.8937 \times 10^{-3}$	$1.2267 \times 10^{-3}$	$5.9612 \times 10^{-4}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0.5$ , $\nu = -1$ , $T = 6$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 4.3985 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0.5$ , $\nu = -1$ , $T = 6$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$3.9877 \times 10^{-1}$	$2.4730 \times 10^{-1}$	$1.4661 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3059 \times 10^{-2}$	$4.4307 \times 10^{-2}$	$2.1244 \times 10^{-2}$	$7.7661 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3451 \times 10^{-3}$	$1.8937 \times 10^{-3}$	$1.2267 \times 10^{-3}$	$5.9612 \times 10^{-4}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0$ , $\nu = 0$ , $T = 20$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 4.3985 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0$ , $\nu = 0$ , $T = 20$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$3.9877 \times 10^{-1}$	$2.4730 \times 10^{-1}$	$1.4661 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3059 \times 10^{-2}$	$4.4307 \times 10^{-2}$	$2.1244 \times 10^{-2}$	$7.7661 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3451 \times 10^{-3}$	$1.8937 \times 10^{-3}$	$1.2267 \times 10^{-3}$	$5.9612 \times 10^{-4}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0$ , $\nu = -1$ , $T = 15$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 4.3985 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = 0$ , $\nu = -1$ , $T = 15$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 5.0000 \times 10^{-2}$				
$R$	15	30	40	50
Relative Error	NA	$3.9877 \times 10^{-1}$	$2.4730 \times 10^{-1}$	$1.4661 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3059 \times 10^{-2}$	$4.4307 \times 10^{-2}$	$2.1244 \times 10^{-2}$	$7.7661 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3451 \times 10^{-3}$	$1.8937 \times 10^{-3}$	$1.2267 \times 10^{-3}$	$5.9612 \times 10^{-4}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = -1$ , $\nu = 0$ , $T = 500$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 4.3985 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = -1$ , $\nu = 0$ , $T = 500$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	NA	$3.9877 \times 10^{-1}$	$2.4730 \times 10^{-1}$	$1.4661 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3059 \times 10^{-2}$	$4.4307 \times 10^{-2}$	$2.1244 \times 10^{-2}$	$7.7661 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3451 \times 10^{-3}$	$1.8937 \times 10^{-3}$	$1.2267 \times 10^{-3}$	$5.9612 \times 10^{-4}$

Parameters: $N = 5$ , $R_\infty = 100$ , $b = 4.4088 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = -1$ , $\nu = -1$ , $T = 400$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	$7.2933 \times 10^{-1}$	$3.9971 \times 10^{-1}$	$2.4788 \times 10^{-1}$	$1.4695 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3255 \times 10^{-2}$	$4.4412 \times 10^{-2}$	$2.1294 \times 10^{-2}$	$7.7844 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3530 \times 10^{-3}$	$1.8982 \times 10^{-3}$	$1.2296 \times 10^{-3}$	$5.9753 \times 10^{-4}$

Parameters: $N = 25$ , $R_\infty = 100$ , $b = 4.3985 \times 10^{-1}$ , $c = -6.6320 \times 10^{-2}$ , $\alpha = -1$ , $\nu = -1$ , $T = 400$ , $h = 1.2500 \times 10^{-1}$ , $\Delta t = 2.5000 \times 10^{-1}$				
$R$	15	30	40	50
Relative Error	NA	$3.9877 \times 10^{-1}$	$2.4730 \times 10^{-1}$	$1.4661 \times 10^{-1}$
$R$	60	70	80	90
Relative Error	$8.3059 \times 10^{-2}$	$4.4307 \times 10^{-2}$	$2.1244 \times 10^{-2}$	$7.7661 \times 10^{-3}$
$R$	95	97	98	99
Relative Error	$3.3451 \times 10^{-3}$	$1.8937 \times 10^{-3}$	$1.2267 \times 10^{-3}$	$5.9612 \times 10^{-4}$

## B - Numerical Codes

The Matlab codes provided in the following Appendix were those utilised in the numerical experiments of Chapter 7.

### numfrag.m

The following code implements the numerical method devised in Chapter 4 for the mixed fragmentation model provided in Chapter 7, Section 7.2.

```

1  function [frag,uDn,uCn,out] = ...
        numfrag(N,R,Ih,T,M,Alpha,Nu,b,c,TMC,MEC)
2
3  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
4  % INPUTS
5  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
6
7  % N      - The discrete/continuous boundary
8  % R      - The continuous regime upper interval cut-off
9  % Ih     - The continuous mass mesh parameter(Ih+1 evenly spaced
10 %         mesh points)
11 % T      - The upper end limit of our time interval
12 % M      - The time partition parameter (M+1 evenly spaced mesh
13 %         points)
14 % Alpha  - The fragmentation rate parameter  $a(x)=x^{\text{alpha}}$ 
15 % Nu     - The selection parameter  $b(x|y)=(\text{Nu}+2)x^{\text{Nu}}/y^{\{\text{Nu}+1\}}$ 
16 % b,c    - Parameters for IC  $b*\exp(c*x)$ 
17 % TMC    - Plot total mass evolution chart, yes/no = 1/0
18 % MEC    - Plot mass distribution evolution chart, yes/no = 1/0
19
20 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
21 % CONSTRUCTING THE MASS AND TIME MESH
22 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
23
24 xd = 1:N;                                %discrete regime integer mass vector
25 xc = linspace(N,R,Ih+1);                 %continuous regime mesh point vector
26
27 %computing the continuous mass interval midpoints
28 xcm = (xc(2:Ih+1)+xc(1:Ih))/2;
29
30 %computing the continuous mass interval lengths
31 dxc = xc(2:Ih+1)-xc(1:Ih);
32
33 %computing timestep
34 dt=T/M;
35
36 %time vector
37 time = linspace(0,T,M+1);
38
39 %computing xi times delta xi for use in mass calculations

```

```

40 xcmdxc = xcm.*dxc;
41
42 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
43 % MODEL SPECIFICATION
44 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
45
46 %computing average values of the continuous fragmentation rate
47 %a(x) over each of the Ih intervals
48 A=zeros(1,Ih);
49 for i=1:Ih
50     A(i)=integral(@(v) frag_rate(v,Alpha),xc(i),xc(i+1))/dxc(i);
51 end
52
53 %computing average values of the continuous selection function
54 %b(x|y) over each of the Ih^2 regions
55 B=zeros(Ih,Ih);
56 for j=1:Ih
57     wl = xc(j); wu = xc(j+1);
58     for i=1:Ih
59         vl = xc(i); vu = xc(i+1);
60         IntB=integral2(@(v,w) c2c_select(v,w,Nu),vl,vu,wl,wu);
61         B(i,j)=IntB/(dxc(i)*dxc(j));
62     end
63 end
64
65 %computing average values of the mixed selection functions
66 %bi(y) over each of the Ih intervals for i=1,...,N
67 BCD=zeros(N,Ih);
68 for i=1:N
69     k = i;
70     for j=1:Ih
71         IntBCD=integral(@(v) c2d_select(v,Nu,k),xc(j),xc(j+1));
72         BCD(i,j)=IntBCD/dxc(j);
73     end
74 end
75
76 %discrete fragmentation rates ai for particles of size i=1,2,...,N
77 ad = zeros(1,N);
78 for i=2:N
79     ad(i)=frag_rate(i);
80 end
81
82 %discrete selection values bij for i,j=1,2,...,N
83 bd = zeros(N,N);
84 for i=1:N
85     for j=1:N
86         bd(i,j)=2/(j-1);
87     end
88 end
89
90 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
91 % CALCULATING APPROXIMATE SOLUTIONS

```

```

92 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
93
94 %initialising our solution matrices
95 uDn=zeros(M+1,N); uCn=zeros(M+1,Ih);
96
97 %computing average values of the initial continuous mass
98 %distribution over the Ih intervals
99 for i=1:Ih
100     uCn(1,i) = integral(@(v)IC(v,b,c),xc(i),xc(i+1))/dxc(i);
101 end
102
103 %initial mass distribution for the discrete regime
104 for i=1:N
105     uDn(1,i) = IC(i,b,c);
106 end
107
108 %calculating regularly used quantities
109 Adxc = A.*dxc;
110 dtAxcm = dt*A./xcm;
111
112 stored = zeros(1,Ih);
113 parfor i=1:Ih
114     stored(i) = dot((1:N),BCD(1:N,i));
115 end
116
117 %computing the approximate solutions for subsequent times
118 for n=2:M+1
119
120     %computing the approximate flux term
121     flux=zeros(1,Ih+1);
122     temp2 = Adxc.*uCn(n-1,:);
123
124     parfor i=2:Ih
125         temp=zeros(1,Ih);
126         for j=i:Ih
127             temp(j)=temp2(j)*dot(xcmdxc(1:i-1),B(1:i-1,j));
128         end
129         flux(i)=sum(temp(i:Ih));
130     end
131
132     %computing approximate sink term
133     sink = dtAxcm.*uCn(n-1,:).*stored;
134
135     %computing the continuous regime approximations
136     uCn(n,:) = uCn(n-1,:) + dt*(flux(2:Ih+1) - flux(1:Ih))./xcmdxc - sink;
137
138     %computing the discrete regime approximations
139     source=zeros(1,N);
140     gain=zeros(1,N);
141     for i=1:N
142
143         %computing source term for mass from the cont. mass regime

```

```

144     temp = Adxc(1:Ih).*BCD(i,1:Ih);
145     source(i) = dt*dot(temp(1:Ih),uCn(n-1,1:Ih));
146
147     %computing fragmentation gain term for particles <N
148     if i < N
149         temp = ad(i+1:N).*bd(i,i+1:N);
150         gain(i)=dt*dot(temp,uDn(n-1,i+1:N));
151     end
152
153 end
154
155 %computing the discrete regime approximations
156 uDn(n,:)=(1-dt*ad).*uDn(n-1,:)+gain+source;
157 end
158
159 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
160 % MASS CALCULATIONS
161 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
162
163 %initialising mass vectors
164 dMASS=zeros(1,M+1);
165 cMASS=zeros(1,M+1);
166 for n = 1:M+1
167     dMASS(n) = dot(uDn(n,:),xd);           %discrete regime mass
168     cMASS(n) = dot(uCn(n,:),xcmdxc);     %continuous regime mass
169 end
170 MASS=dMASS+cMASS;                       %total mass
171
172 %initialising mass change vector
173 DELTAMASS=zeros(1,M);
174
175 %calculating change in mass between timesteps
176 for n=1:M
177     DELTAMASS(n)=abs(MASS(n+1)-MASS(n));
178 end
179
180 %check sum of total mass changes
181 frag = sum(DELTAMASS);
182
183 %parameters required for truncerror.m
184 out = {dxc(1),xcm,dt,MASS(1),N};
185
186 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
187 % Particle Number Calculations
188 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
189
190 %initialising particle numbers vector
191 Pno=zeros(1,M+1);
192
193 for n = 1:M+1
194     dPno = sum(uDn(n,:));
195     cPno = dot(uCn(n,:),dxc);

```

```

196     Pno(n)=dPno+cPno;
197 end
198
199 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
200 % PLOTTING
201 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
202 close all
203
204 %plotting total mass charts%
205 if TMC == 1
206     figure(1)
207     movegui(figure(1), 'northeast');
208     plot(time,MASS)
209     title('Mass Evolution')
210     xlabel('Time')
211     ylabel('Mass')
212     hold('on')
213     plot(time,dMASS,'k')
214     plot(time,cMASS,'r')
215     plot(time,mMASS,'m')
216     legend('Total Mass','Disc. Mass','Cont. Mass','Mono. ...
           Mass','Location','best');
217     hold('off')
218 end
219
220 %plotting particle numbers chart%
221 if TMC == 1
222     figure(2)
223     movegui(figure(2), 'southeast');
224     title('Particle Number Evolution')
225     xlabel('Time')
226     ylabel('No. of Particles')
227     hold('on')
228     plot(time,Pno,'k')
229     legend('Particle Numbers','Location','best');
230     hold('off')
231 end
232
233 %plotting evolution charts
234 if MEC == 1
235     upper = 1.1*R;
236     for n = 3:M+3
237         figure(n)
238         movegui(figure(n), 'northwest');
239         scatter(xd,uDn(n-2,:), '*','b')
240         hold('on')
241         plot(xcm,uCn(n-2,:), 'b')
242         title('Particle Mass Distribution')
243         xlabel('Particle Size')
244         ylabel('Concentration')
245         legend('Disc. Particle Mass','Cont. Particle ...
           Mass','Location','northeast');

```

```
246         xlim([0 upper])
247         hold('off')
248     end
249 end
250
251 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
252 % MODEL CONFIGURATION FUNCTIONS AND ICs
253 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
254
255 %Continuous fragmentation rate
256
257 function out = frag_rate(v,Alpha)
258
259 out = v.^Alpha;
260
261 %Continuous to continuous resulting distribution
262
263 function out = c2c_select(v,w,Nu)
264
265 out = (Nu+2)*(v.^Nu)./(w.^(Nu+1));
266
267 %Continuous to discrete resulting distribution
268
269 function out = c2d_select(v,Nu,k)
270
271 out = (k.^(Nu+2)-(k-1).^(Nu+2))./(k*(v.^(Nu+1)));
272
273 %Continuous regime initial condition
274
275 function out = IC(v,b,c)
276
277 out = b*exp(c*v);
```



```

45 %discrete fragmentation rates ai for particles of size i=1,2,...,N
46 ad = zeros(1,N);
47 for i = 2:N
48     ad(i) = i^Alpha;
49 end
50
51 %discrete selection values bij for i,j=1,2,...,N
52 bd = zeros(N,N);
53 for i = 1:N-1
54     for j = i+1:N
55         bd(i,j) = 2/(j-1);
56     end
57 end
58 for i = 1:N
59     bd(i,i) = -1;
60 end
61
62 C = zeros(N,N);
63 for i = 1:N
64     for j = 1:N
65         C(i,j) = ad(j)*bd(i,j);
66     end
67 end
68
69 %continuous to discrete resulting distribution
70 bdC = zeros(N,1);
71 for i = 1:N
72     bdC(i) = (i^(nu+2)-(i-1)^(nu+2))/i;
73 end
74
75 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
76 % CALCULATING SOLUTIONS ON MESH POINTS
77 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
78
79 %initialising our solution matrices
80 uDe = zeros(M+1,N); uCe = zeros(M+1,Ih);
81
82 %initial mass distribution for the continuous regime
83 for j = 1:Ih
84     uCe(1,j) = IC(xcm(j),b,c);
85 end
86
87 %computing the initial mass in the continuous regime
88 cont_mass = integral(@(y) ICmass(y,b,c),N,R);
89
90 %calculating the mass distribution for the continuous regime
91 %for subsequent times
92 for n = 2:M+1
93     t = time(n);
94     for j = 1:Ih
95         uCe(n,j) = ucont(xcm(j),t,para);
96     end

```

```

97 end
98
99 %initial mass distribution for the discrete regime
100 for i = 1:N
101     uDe(1,i) = IC(i,b,c);
102 end
103 i_state = uDe(1,:);
104
105 %computing the initial mass in the disc. regime
106 disc_mass = dot((1:N),i_state);
107
108 %calculating the mass distribution for the discrete regime
109 %for subsequent times
110
111 ME = zeros(N,N,M);
112
113 parfor n = 1:M
114     t1 = time(n); tu = time(n+1);
115     ME(:, :, n) = ...
116         integral(@ (s) Mat_exp(s,C,para),t1,tu,'ArrayValued',1);
117
118 T2 = T/2;
119
120 parfor n = 2:M+1
121     Matexp = sum(ME(:, :, 1:(n-1)), 3);
122     gain = expm((time(n)-T2)*C)*Matexp*bdC;
123     uDe(n, :) = expm(time(n)*C)*transpose(i_state)+gain;
124 end
125
126 %normalising divisor for relative error calculations
127 norm_div = T*(disc_mass+cont_mass);
128
129 %parameters required for fragerror.m
130 out = {dx,xcm,dt,norm_div,N};
131
132 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
133 % PLOTTING
134 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
135 close all
136
137 %plotting evolution charts
138 if MEC == 1
139     upper = 1.1*R;
140     for n = 1:M+1
141         figure(n)
142         movegui (figure(n), 'northwest');
143         scatter(xd,uDe(n, :), '*','b')
144         hold('on')
145         plot(xcm,uCe(n, :), 'b')
146         title(['Particle Mass Distribution at time t = ' ...
147             num2str(time(n)) ])

```

```

147         xlabel('Particle Size')
148         ylabel('Concentration')
149         legend('Disc. Particle Mass','Cont. Particle ...
           Mass','Location','northeast');
150         xlim([0 upper])
151         hold('off')
152     end
153 end
154
155 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
156 % SUBFUNCTIONS
157 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
158
159 % Initial conditions for cont. regime
160
161 function out = IC(y,b,c)
162
163 out = b*exp(c*y);
164
165 % Integrand for initial cont. mass calculation
166
167 function out = ICmass(y,b,c)
168
169 out = IC(y,b,c).*y;
170
171 % Computatation of confluent hypergeometric function 1F1
172
173 function out = hyperg(Y,x,t,para)
174
175 %-----%
176 % Adapted from code by John Pearson, University of Oxford, %
177 % as part of the MSc dissertation: %
178 % 'Computation of Hypergeometric Functions' %
179 %-----%
180
181 Alpha = para(3); m = para(5);
182
183 a = 1-m;
184 b = 2;
185 tol = 10^(-15);
186
187 len = length(Y);
188 out = zeros(1,len);
189
190 for g = 1:len
191     y = Y(g);
192     z = t*(x^Alpha-y^Alpha);
193
194     % Initialise a1, vector of individual terms, and b1,
195     % which stores the sum of the computed terms up to
196     % that point
197     a1=zeros(1,1);

```

```

198     a1(1)=1;b1=1;
199
200     if abs(z)<50
201
202         for j=1:500
203             % Compute current entry of a1 in terms of last
204             a1(j+1)=(a+j-1)/(b+j-1)*z/j*a1(j);
205             % Update the sum of computed terms up to that point
206             b1=b1+a1(j+1);
207             % Apply stopping criterion, as detailed in Section 3.2
208             if abs(a1(j))/abs(b1)<tol && abs(a1(j+1))/abs(b1)<tol
209                 break
210             end
211
212             % If 500 terms have been computed without stopping
213             % criterion being satisfied, state this
214             if (j==500)
215                 [' ' num2str(j) ' terms computed'] %#ok<*NOPRT>
216                 return
217             end
218         end
219
220         % If stopping criterion has been satisfied, return sum
221         % of terms computed, i.e return b1
222         out(g) = b1;
223
224     else
225
226         for j=1:500
227             % Update a1(j) and b1 in terms of previously
228             % computed a1(j-1) and b1
229             a1(j+1)=(b-a+j-1)*(-a+j)/j/z*a1(j);
230             b1=b1+a1(j+1);
231             % If stopping criterion is satisfied
232             if abs(a1(j))/abs(b1)<tol && abs(a1(j+1))/abs(b1)<tol
233                 break
234             end
235             % If 500 terms have been computed before stopping
236             % criterion has been satisfied, state this
237             if (j==500)
238                 [' ' num2str(j) ' terms computed']
239                 return
240             end
241         end
242
243         % Initialise c1, which represents current term, and d1,
244         % which represents sum of all terms computed thus far,
245         % for second series in (3.23) and (3.24)
246         c1=zeros(1,1);
247         c1(1)=1;d1=1;
248
249         for k=1:500

```

```

250     % Update c1 and d1
251     c1(k+1)=(a+k-1)*(a-b+k)/k/(-z)*c1(k);
252     d1=d1+c1(k+1);
253     % Stopping criterion
254     if abs(c1(k))/abs(d1)<tol && abs(c1(k+1))/abs(d1)<tol
255         break
256     end
257     % Specify if 500 terms computed
258     if (k==500)
259         [' ' num2str(k) ' terms computed']
260         return
261     end
262 end
263
264 % Take last terms computed
265 h1=b1;h2=d1;
266
267 % Compute relevant Gamma functions using cgama.m [71]
268 [gr1,gi1]=cgama(b,0,1);
269 [gr2,gi2]=cgama(a,0,1);
270 [gr3,gi3]=cgama(b-a,0,1);
271
272 % Compute (3.23) or (3.24)
273 if (zr>0)
274     h3=(gr1+gi1*1i)*exp(z)*z^(a-b)/(gr2+gi2*1i)*h1...
275         +exp(pi*1i*a)*z^(-a)/(gr3+gi3*1i)*h2;
276 elseif (zr<0)
277     h3=(gr1+gi1*1i)*(exp(z)*z^(a-b)/(gr2+gi2*1i)*h1...
278         +exp(-pi*1i*a)*z^(-a)/(gr3+gi3*1i)*h2);
279 end
280
281 % Take real part if Im(a)=Im(b)=Im(z)=0, otherwise
282 % simply take what has been computed
283
284 out(g) = real(h3);
285
286 end
287 end
288
289 % Continuous regime solution
290
291 function out = ucont(x,t,para)
292
293 R = para(2); Alpha = para(3); nu = para(4);
294 m = para(5); b = para(7); c = para(8);
295
296 integrand = @(y) (y.^(Alpha-nu-1)).*IC(y,b,c).*hyperg(y,x,t,para);
297
298 int = integral(integrand,x,R);
299
300 out = exp(-t*(x.^Alpha))*(IC(x,b,c)+(m*Alpha*t)*(x.^nu)*int);
301

```

```
302 % Continuous regime solution for integration in calculation
303 % of discrete regime solution
304
305 function out = ucontint(Y,s,para)
306
307 R = para(2); Alpha = para(3); nu = para(4);
308 m = para(5); b = para(7); c = para(8);
309
310 out = zeros(1,length(Y));
311
312 for j = 1:length(Y)
313
314     y = Y(j);
315
316     integrand=@(v) (v.^(Alpha-nu-1)).*IC(v,b,c).*hyperg(v,y,s,para);
317
318     int = integral(integrand,y,R);
319
320     out(j)=exp(-s*(y.^Alpha))*(IC(y,b,c)+(m*Alpha*s)*(y.^nu)*int);
321
322 end
323
324 % Matrix exponential integrand for computation of discrete
325 % regime solution
326
327 function out = Mat_exp(S,C,para)
328
329 N = para(1); R = para(2); T = para(6);
330
331 out = zeros(N,N,length(S));
332
333 T2 = T/2;
334
335 for j = 1:length(S)
336
337     s = S(j);
338
339     integrand = @(y) (y.^(Alpha-nu-1)).*ucontint(y,s,para)
340
341     integralterm = integral(integrand,N,R);
342
343     out(:, :, j) = expm((T2-s)*C).*integralterm;
344
345 end
```

**numerror.m**

The following code computes the relative error of the numerical approximations from numfrag.m against a fine mesh evaluation of the exact solution computed using exactfrag.m.

```

1 function rel_error = numerror(uDn,uCn,uDe,uCe,out)
2
3 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
4 % INPUTS
5 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
6 %
7 % uDn - discrete regime numerical approx. values
8 % uCn - continuous regime numerical approx. values
9 % uDe - discrete regime exact solution values
10 % uCe - continuous regime exact solution values
11 % out - list of required parameters
12 %
13 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
14
15 % Extracting the parameters from list
16
17 dx = out{:,1}; xcm = out{:,2}; dt = out{:,3};
18 norm_div = out{:,4}; N = out{:,5};
19
20 % Computing the scale up factor for the numerical approx array
21
22 [tlow,xlow] = size(uCn); [thigh,xhigh] = size(uCe);
23
24 tfactor = (thigh-1)/(tlow-1); xfactor = xhigh/xlow;
25
26 % Shaping the numerical approx. and exact solution arrays
27 % to match in size
28
29 uDn_enlarged = repelem(uDn(1:end-1,:),tfactor,1);
30 uDe_short = uDe(1:end-1,:);
31 uCn_enlarged = repelem(uCn(1:end-1,:),tfactor,xfactor);
32 uCe_short = uCe(1:end-1,:);
33
34 % Computing the norm of the discrete regime error
35
36 D_error = dt*dot((1:N),sum(abs(uDe_short-uDn_enlarged)));
37
38 % Computing the norm of the continuous regime error
39
40 C_error = dt*dx*dot(xcm,sum(abs(uCe_short-uCn_enlarged)));
41
42 % Computing the relative error of the approximation
43
44 rel_error = (D_error+C_error)/norm_div;

```

**Init\_fit.m**

The following code computes the parameters  $(b, c)$  for the initial mass distributions  $d_{0i} = be^{ci}$  and  $c_0(x) = be^{cx}$ . The value of  $c$  is chosen so that the mass over the truncated domain up to  $R$ , accounts for a proportion  $p$  of the mass over the infinite domain. This is achieved using the bisection method. The value of  $b$  is then selected in a manner that the total mass associated with the truncated distribution is equal to  $M$ .

```

1 function [b,c] = Init_fit(N,R,p,TM,tol,c0)
2
3 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
4 % INPUTS
5 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
6 %
7 % N   - The discrete/continuous boundary
8 % R   - The continuous regime upper interval cut-off
9 % p   - Proportion of mass accounted for in the truncation
10 % TM  - Mass in the truncated system
11 % c0  - Search interval endpoint, [c0,c1], c0<0, initially c1=0
12 % tol - Tolerance, terminate when |c1-c0|<tol
13 %
14 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
15
16 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
17 % Solving for c using the bisection method
18 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
19
20 para = [N,R,p];    %vector of parameters
21 c1 = 0;
22 check = tol+1;
23
24 while check>tol
25
26     range = linspace(c0,c1,100);
27     L = length(range);
28
29     Fvals = zeros(1,L);
30     for j = 1:L
31         Fvals(j) = F(range(j),para);
32     end
33
34     clower = range(1:end-1); cupper = range(2:end);
35     lower = Fvals(1:end-1); upper = Fvals(2:end);
36
37     Product = lower.*upper;
38
39     Rootfind = zeros(1,L-1);
40     for j = 1:L-1
41         if Product(j)<0

```

```

42         Rootfind(j)=1;
43     end
44 end
45
46     ind = find(Rootfind,1,'last');
47
48     c0 = clower(ind);
49     c1 = cupper(ind);
50     check = abs(c0-c1);
51
52 end
53
54 c = (c0+c1)/2;
55
56 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
57 % Solving for b via mass calculations
58 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
59
60 % calculating mass within discrete regime
61 xd = 1:N;
62 disc_mass = dot(xd,exp(c*xd));
63
64 % calculating mass within continuous regime
65 cont_mass = (exp(c*R)*(c*R-1)+exp(c*N)*(1-c*N))/c^2;
66
67 % solving for scaling constant b so that mass = M
68 b = TM/(disc_mass+cont_mass);
69
70 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
71 % PLOTTING
72 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
73
74 % evaluating discrete regime values
75 uD = zeros(1,N);
76 for i=1:N
77     uD(i)=IC(i,b,c);
78 end
79
80 % evaluating continuous regime values
81 xc = linspace(N,R,100);
82 uC = zeros(1,length(xc));
83 for i=1:length(xc)
84     uC(i)=IC(xc(i),b,c);
85 end
86
87 %plotting initial mass distribution chart
88 close all
89
90 upper = 1.1*R;
91 hold('on')
92 scatter(xd,uD,'*', 'b')
93 plot(xc,uC, 'b')

```

```
94 title('Initial Particle Mass Distribution')
95 xlabel('Particle Mass')
96 ylabel('Concentration')
97 legend('Disc. Particle Mass','Cont. Particle ...
      Mass','Location','northeast');
98 xlim([0 upper])
99 hold('off')
100
101 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
102 % SUBFUNCTIONS
103 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
104
105 % Function F for which we require the root c, F(c)=0
106
107 function out = F(c,para)
108
109 N = para(1); R = para(2); p = para(3);
110
111 i=1:N;
112
113 Q1 = (1-p)*sum((c^2*i).*exp(c*i));
114 Q2 = (p-1)*(c*N-1)*exp(c*N);
115 Q3 = (c*R-1)*exp(c*R);
116
117 out = Q1+Q2+Q3;
118
119 % Initial state for plotting
120
121 function out = IC(y,b,c)
122
123 out = b*exp(c*y);
```

**truncerror.m**

The following code computes the relative error between two numerical approximations produced by `numfrag.m`, for different choices of the parameter  $R$ .

```

1 function rel_error = truncerror(uDnr, uCnr, uDnR, uCnR, out)
2
3 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
4 % INPUTS
5 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
6 %
7 % uDnr - discrete regime values with small R
8 % uCnr - continuous regime values with small R
9 % uDnR - discrete regime values with large R
10 % uCnR - continuous regime values with Large R
11 % out - list of required parameters
12 %
13 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
14
15 % Extracting the parameters from list
16 dx = out(:,1);
17 xcm = out(:,2);
18 dt = out(:,3);
19 norm_div = out(:,4);
20 N = out(:,5);
21
22 %removing last time step as not required for [0,T)
23 uDnr = uDnr(1:end-1, :);
24 uCnr = uCnr(1:end-1, :);
25 uDnR = uDnR(1:end-1, :);
26 uCnR = uCnR(1:end-1, :);
27
28 %Resizing the matrices of solution values to have common size
29 [M,upper] = size(uCnR); [~,lower] = size(uCnr);
30
31 temp = zeros(M, upper);
32 temp(:,1:lower) = uCnr; uCnr = temp;
33
34 %Computing the norm of the discrete regime error
35
36 D_error = dt*dot((1:N), sum(abs(uDnR-uDnr)));
37
38 %Computing the norm of the continuous regime error
39
40 C_error = dt*dx*dot(xcm, sum(abs(uCnR-uCnr)));
41
42 %Computing the relative error of the truncated solution
43
44 rel_error = (D_error+C_error)/norm_div;

```

## C - Justification for Leibniz's Rule

In Chapter 4, when reformulating equation (4.1) as (4.2), we utilised Leibniz's rule for differentiating under the integral in order to justify the equivalence of the two equations. It is not immediately clear that this operation is entirely rigorous, therefore we now prove from first principles the equivalence of the two forms, assuming that for each  $t$  the function  $u_C^R(x, t)$  is integrable over  $(N, R)$  with respect to  $x$ .

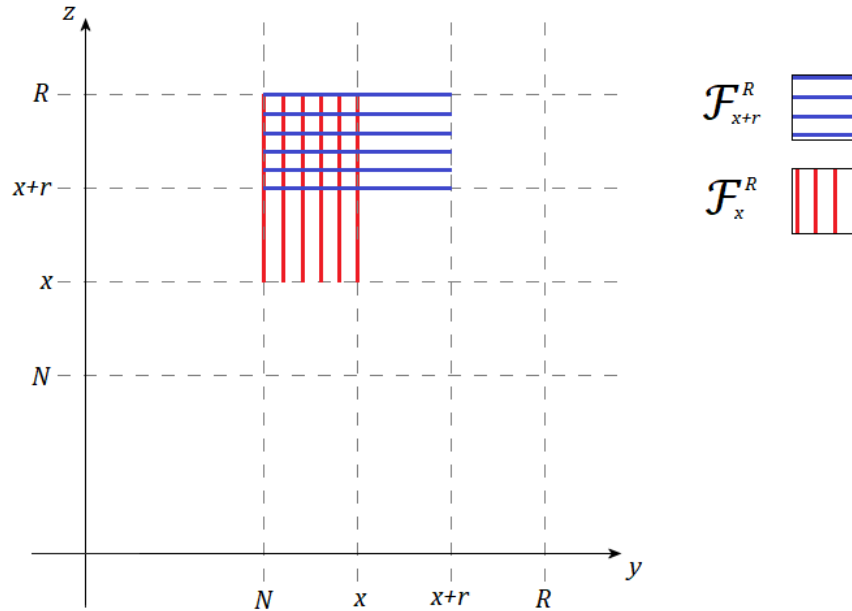
Let us consider the derivative  $\frac{\partial \mathcal{F}^R(v)}{\partial x}$  appearing on the right-hand side of (4.2), where  $v(x, t) = xu_C^R(x, t)$  and

$$\mathcal{F}^R(v) = \int_x^R \int_N^x ya(z)b(y|z)u_C^R(z, t) dy dz, \text{ for } N < x < R.$$

Writing  $\mathcal{F}_x^R$  to denote the mass flux  $\mathcal{F}^R(v)$  at a point  $x \in (N, R)$  and taking  $r > 0$  to be such that  $x + r \in (N, R)$ , we consider

$$\begin{aligned} \frac{\mathcal{F}_{x+r}^R - \mathcal{F}_x^R}{r} &= \frac{1}{r} \int_{x+r}^R \int_N^{x+r} ya(z)b(y|z)u_C^R(z, t) dy dz \\ &\quad - \frac{1}{r} \int_x^R \int_N^x ya(z)b(y|z)u_C^R(z, t) dy dz. \end{aligned}$$

The two overlapping regions of integration can be seen represented geometrically in the diagram below.



Rewriting our integrals, taking account of the overlapping region where they cancel each other out, we arrive at the following:

$$\begin{aligned} \frac{\mathcal{F}_{x+r}^R - \mathcal{F}_x^R}{r} &= \frac{1}{r} \int_{x+r}^R \int_x^{x+r} ya(z)b(y|z)u_C^R(z,t) dy dz \\ &\quad - \frac{1}{r} \int_x^{x+r} \int_N^x ya(z)b(y|z)u_C^R(z,t) dy dz. \end{aligned} \quad (\text{C.1})$$

Taking the first of these double integrals, we may write it as

$$\int_x^R \chi_{(x+r,R)}(z)a(z)u_C^R(z,t) \frac{1}{r} \int_x^{x+r} yb(y|z) dy dz. \quad (\text{C.2})$$

Firstly, let us note that the integrand may be bounded in a straightforward manner by

$$\alpha(R)u_C^R(z,t)R\beta(R),$$

as a result of the  $L_{\infty,loc}$  nature of the functions  $a$  and  $b$ . Furthermore, from our assumption regarding  $u_C^R$ , this bound can be seen to be integrable over  $(x,R)$ . Turning our attention to the inner integral of (C.2), for fixed  $z \in (x,R)$  let us denote by  $H_{x,z}(y)$  a function defined to take the value  $yb(y|z)$  for  $y \in [x, x+r)$ , which is then reflected symmetrically about the line  $y = x$ . Having done so, we may express the inner integral of (C.2) like so:

$$\frac{1}{r} \int_x^{x+r} yb(y|z) dy = \frac{1}{2} \frac{2}{2r} \int_{x-r}^{x+r} H_{x,z}(y) dy \rightarrow H_{x,z}(x) = xb(x|z) \quad \text{as } r \searrow 0.$$

Owing to  $b \in L_{\infty,loc}$  and the Lebesgue differentiation theorem (Theorem 2.1.4), this convergence is valid for almost all  $x$  and  $z$ . We shall utilise this method a number of times in the upcoming material, when we shall refer to it as the ‘reflection procedure’ rather than recounting the same details. Hence the integrand from the outer integral of (C.2) converges pointwise almost everywhere to

$$xa(z)b(x|z)u_C^R(z,t).$$

An application of the Lebesgue dominated convergence theorem then yields:

$$\frac{1}{r} \int_{x+r}^R \int_x^{x+r} ya(z)b(y|z)u_C^R(z,t) dy dz \rightarrow \int_x^R xa(z)b(x|z)u_C^R(z,t) dz, \quad (\text{C.3})$$

as we let  $r \searrow 0$ . Examining the second of the integrals from (C.1), we may rewrite it as

$$\frac{1}{r} \int_x^{x+r} a(z)u_C^R(z,t) \int_N^x yb(y|z) dy dz. \quad (\text{C.4})$$

From the outer limits of integration we have  $x \leq z$ ; then, utilising the mass conservation condition (3.3), we may bound the inner integral of (C.4) like so:

$$\int_N^x yb(y|z) dy \leq \int_N^z yb(y|z) dy \leq z.$$

This in turn allows us to bound the integrand of the outer integral by

$$\alpha(R)u_C^R(z, t)R,$$

which is integrable as a result of our assumption regarding  $u_C^R$ . Applying the reflection procedure to (C.4) and letting  $r \searrow 0$ , we obtain

$$\begin{aligned} \frac{1}{r} \int_x^{x+r} a(z)u_C^R(z, t) \int_N^x yb(y|z) dy dz &\rightarrow a(x)u_C^R(x, t) \int_N^x yb(y|x) dy \\ &= a(x)u_C^R(x, t) \left( x - \sum_{j=1}^N j b_j(x) \right), \end{aligned}$$

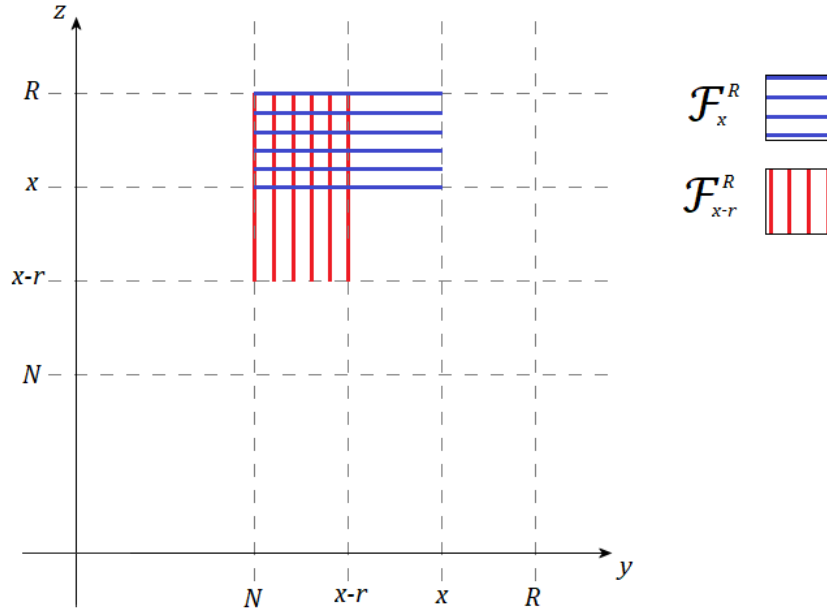
where the equality comes as a result of condition (3.3). Combining this with (C.3) we get

$$\begin{aligned} \lim_{r \rightarrow 0^+} \frac{\mathcal{F}_{x+r}^R - \mathcal{F}_x^R}{r} &= \int_x^R xa(z)b(x|z)u_C^R(z, t) dz - a(x)u_C^R(x, t) \left( x - \sum_{j=1}^N j b_j(x) \right) \\ &= x \left( -a(x)u_C^R(x, t) + \int_x^R a(z)b(x|z)u_C^R(z, t) dz \right) + \underbrace{\frac{a(x)}{x} \sum_{j=1}^N j b_j(x) x u_C^R(x, t)}_{=S(xu_C^R)}. \end{aligned}$$

Establishing the right-hand derivative of  $\mathcal{F}^R(v)$  at  $x \in (N, R)$ . For the left derivative, let  $x \in (N, R)$  be fixed and  $r > 0$  be such that  $x - r \in (N, R)$ , then we consider

$$\begin{aligned} \frac{\mathcal{F}_x^R - \mathcal{F}_{x-r}^R}{r} &= \frac{1}{r} \int_x^R \int_N^x ya(z)b(y|z)u_C^R(z, t) dy dz \\ &\quad - \frac{1}{r} \int_{x-r}^R \int_N^{x-r} ya(z)b(y|z)u_C^R(z, t) dy dz. \end{aligned}$$

As before, the two double integrals have an area of overlap in their regions of integration; this overlap can be seen in the diagram below.



Accounting for the overlap, where the two integrals cancel each other out, we end up with

$$\begin{aligned} \frac{\mathcal{F}_x^R - \mathcal{F}_{x-r}^R}{r} &= \frac{1}{r} \int_x^R \int_{x-r}^x ya(z)b(y|z)u_C^R(z, t) dy dz \\ &\quad - \frac{1}{r} \int_{x-r}^x \int_N^{x-r} ya(z)b(y|z)u_C^R(z, t) dy dz. \end{aligned} \quad (\text{C.5})$$

Taking the first of these double integrals we may rewrite it in the following way:

$$\int_x^R a(z)u_C^R(z, t) \frac{1}{r} \int_{x-r}^x yb(y|z) dy dz. \quad (\text{C.6})$$

The innermost integrand  $yb(y|z)$  is bounded by  $R\beta(R)$ , allowing us to apply the reflection procedure once again to give

$$\frac{1}{r} \int_{x-r}^x yb(y|z) dy \rightarrow xb(x|z) \quad \text{as } r \searrow 0,$$

with this convergence being valid for almost all  $x$  and  $z$ . Furthermore, the integrand from the outer integral of (C.6) may be bounded by the integrable function  $\alpha(R)u_C^R(z, t)R\beta(R)$ , hence we may apply the dominated convergence theorem once again to obtain

$$\frac{1}{r} \int_x^R \int_{x-r}^x ya(z)b(y|z)u_C^R(z, t) dy dz \rightarrow \int_x^R xa(z)b(x|z)u_C^R(z, t) dz. \quad (\text{C.7})$$

With a switch of integration order, which may be justified by Tonelli's theorem, the second integral of (C.5) may be expressed as

$$\int_N \chi_{(N, x-r)}(y) y \frac{1}{r} \int_{x-r}^x a(z) b(y|z) u_C^R(z, t) dz dy. \quad (\text{C.8})$$

By the usual reflection argument, we have:

$$\frac{1}{r} \int_{x-r}^x a(z) b(y|z) u_C^R(z, t) dz \rightarrow a(x) b(y|x) u_C^R(x, t) \quad \text{as } r \searrow 0,$$

for almost all  $x \in (N, R)$  and  $y \in (N, x)$ , which implies that the outer integrand from (C.8) converges pointwise almost everywhere to  $ya(x)b(y|x)u_C^R(x, t)$ . Additionally, this integrand may be bounded by

$$R\alpha(R)\beta(R) \frac{1}{r} \int_{x-r}^x u_C^R(z, t) dz. \quad (\text{C.9})$$

The Lebesgue differentiation theorem and the reflection procedure give us

$$\frac{1}{r} \int_{x-r}^x u_C^R(z, t) dz \rightarrow u_C^R(x, t) \quad \text{as } r \searrow 0.$$

Hence given any  $\epsilon > 0$  we can find a corresponding  $\delta(\epsilon) > 0$ , such that  $r < \delta(\epsilon)$  implies

$$\left| \frac{1}{r} \int_{x-r}^x u_C^R(z, t) dz - u_C^R(x, t) \right| < \epsilon \Rightarrow \frac{1}{r} \int_{x-r}^x u_C^R(z, t) dz < u_C^R(x, t) + \epsilon.$$

Since the convergence used to derive this bound was independent of  $y$ , we may further bound (C.9) by

$$R\alpha(R)\beta(R) (u_C^R(x, t) + \epsilon),$$

which, for almost all  $x$ , must be finite and hence integrable with respect to  $y$  over  $(N, x)$ . The dominated convergence theorem allows us to deduce that

$$\begin{aligned} & \frac{1}{r} \int_{x-r}^x \int_N ya(z)b(y|z)u_C^R(z, t) dy dz \rightarrow \int_N ya(x)b(y|x)u_C^R(x, t) dy \\ & = a(x)u_C^R(x, t) \int_N yb(y|x) dy = a(x)u_C^R(x, t) \left( x - \sum_{j=1}^N j b_j(x) \right), \end{aligned}$$

as we let  $r \searrow 0$ . The final equality is once again a consequence of the mass conservation condition (3.3). Putting this together with (C.5) and (C.7) yields

$$\begin{aligned} \lim_{r \rightarrow 0^+} \frac{\mathcal{F}_x^R - \mathcal{F}_{x-r}^R}{r} &= \int_x^R xa(z)b(x|z)u_C^R(z, t) dy dz - a(x)u_C^R(x, t) \left( x - \sum_{j=1}^N j b_j(x) \right) \\ &= x \left( -a(x)u_C^R(x, t) + \int_x^R a(z)b(x|z)u_C^R(z, t) dz \right) + \underbrace{\frac{a(x)}{x} \sum_{j=1}^N j b_j(x) x u_C^R(x, t)}_{=S(xu_C^R)}. \end{aligned}$$

which gives us the left-hand derivative of  $\mathcal{F}^R(v)$  at  $x \in (N, R)$ . Having determined the left and right derivatives of  $\mathcal{F}^R(v)$  and having found them to be equal, we have therefore established the differentiability of  $\mathcal{F}^R(v)$ , with

$$\frac{\partial \mathcal{F}^R(v)}{\partial x} = x \left( -a(x)u_C^R(x, t) + \int_x^R a(z)b(x|z)u_C^R(z, t) dz \right) + S(xu_C^R),$$

which holds for almost all  $x \in (N, R)$ . Therefore, given a classical solution  $u_C^R(x, t)$  to either one of the formulations (4.1) or (4.2), then provided this solution is integrable with respect  $x$  over  $(N, R)$  for almost all  $t$ , it is then also a solution to the alternative formulation.

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