Mathematical and numerical analysis for coagulation-fragmentation equations

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Abstract

This thesis is devoted to the mathematical and numerical analysis for the continuous coagulation-fragmentation equation. This is a partial integro-differential equation.

There have been several investigations of existence and uniqueness of solutions to the coagulation and binary fragmentation equation with different classes of kernels. However, the case of multiple fragmentation was almost ignored. The first aim of this work is to prove the existence of solutions to the continuous coagulation and multiple fragmentation equation for large classes of kernels. Here we would like to cover those coagulation kernels which are not included in the previous literature for the study of the continuous coagulation equation with multiple fragmentation. It is also of great interest to investigate the uniqueness of solutions. However, in order to prove the uniqueness, we need more restrictive conditions on the kernels.

The second aim is to demonstrate the uniqueness of mass conserving solutions to the continuous coagulation and binary fragmentation equation. In this case, the existence of mass conserving solutions was established in Escobedo et al. [27] for a large class of coagulation kernels with strong fragmentation. This strong fragmentation prevents the occurrence of the gelation phenomenon and gives the existence of mass conserving solutions when the class of coagulation kernels grows beyond linearity. Note that the gelation phenomenon usually leads to solutions which are not mass conserving. Therefore, the proof of uniqueness requires additional growth conditions on the fragmentation kernels.

The third target is to extend the previous existence result for the coagulation and multiple fragmentation equation. In this work we wish to include some classical multiple fragmentation kernels which are not covered in the existence result mentioned above. It should also be remarked that the classes of coagulation kernels are identical to those in the above result.

The next goal is to develop the convergence analysis of sectional methods for solving the non-linear pure coagulation equation. Here we examine the most popular of all sectional methods the fixed pivot technique. We investigate the convergence of the fixed pivot scheme on five different grid types. We found that the scheme is second order accurate on uniform and non-uniform smooth grids while it shows first order accuracy on locally uniform grids. The undesirable result is that the scheme is not convergent on oscillatory and random grids. Finally, we demonstrate practical significance of the mathematical results by performing a few numerical simulations.

The fixed pivot technique gives a consistent over prediction of the solution for the large size particles when applied on coarse grids. To overcome this problem, the cell average technique was introduced which preserves all advantages of the fixed pivot technique and

improves the numerical results. Further, we are also interested to evaluate the order of convergence of the cell average technique for the pure coagulation equation by performing several numerical experiments. Then we compare the numerical results with the result obtained by the fixed pivot technique. This cell average technique yields second order accuracy on uniform, non-uniform smooth and locally uniform grids. The scheme turns into a first order accurate method on oscillatory and random grids. Therefore, the cell average technique experimentally shows one order higher accuracy than the fixed pivot technique for locally uniform, oscillatory and non-uniform random grids. The mathematical proof of this higher order remains an open problem.

Zusammenfassung

Diese Doktorarbeit ist der mathematischen und numerischen Analysis der Gleichung des kontinuierlichen Koagulations- und Fragmentationsprozesses gewidmet. Dieses ist eine partielle Integro-Differential-Gleichung.

Es gibt zahlreiche Untersuchungen zur Existenz und Eindeutigkeit von Lösungen einer Koagulations- und binären Fragmentationsgleichung mit unterschiedlichen Klassen von Kernfunktionen. Der Fall der mehrfachen Fragmentation ist dagegen noch nicht eingehend untersucht worden. Das erste Ziel dieser Arbeit ist ein Existenznachweis für Lösungen einer kontinuierlichen Koagulations- und mehrfachen Fragmentationsgleichung für eine grosse Klasse von Kernfunktionen. Wir möchten hier solche Koagulationskerne behandeln, die in der bisherigen Literatur für das Studium einer kontinuierlichen Koagulations- und mehrfachen Fragmentationsgleichung nicht berücksichtigt wurden. Auch ein Eindeutigkeitsnachweis für solche Lösungen ist in diesem Zusammenhang von grossem Interesse. Jedoch müssen wir für diesen Eindeutigkeitsnachweis einschränkendere Bedingungen an die Kernfunktionen stellen.

Das zweite Ziel ist der Eindeutigkeitsnachweis für Lösungen einer Koagulations- und binären Fragmentationsgleichung mit Massenerhalt. In diesem Fall wurde die Existenz massenerhaltender Lösungen von Escobedo et al. [27] für eine grosse Klasse von Koagulationskernen mit starker Fragmentation gezeigt. Die starke Fragmentation verhindert das Auftreten von Gelbildungsprozessen und liefert die Existenz massenerhaltender Lösungen falls für die Klasse der Koagulationskerne ein Wachstum vorliegt, das stärker als linear ist. Man beachte dabei, dass Prozesse mit Gelbildung im allgemeinen zu Lösungen führen, die den Massenerhalt verletzen. Daher werden für den Eindeutigkeitsnachweis zusätzliche Wachstumsbedingungen an die Fragmentationskerne gestellt.

Das dritte Ziel ist das vorher gewonnene Existenzresultat auf Gleichungen mit Koagulations- und mehrfache Fragmentation zu erweitern. In diesem Teil konnten wir einige mehrfache Fragmentationskerne abdecken, die in der Literatur noch nicht behandelt wurden. Die Koagulationskerne sind die Gleichen wie im vorhergehenden Teil.

Das nächste Ziel ist die Entwicklung einer Konvergenzanalysis von Diskretisierungsmethoden zur Lösung der nichtlinearen reinen Koagulationsgleichung. Zuerst untersuchen wir die populärste Methode, nämlich die "fixed pivot"-Technik. Hier untersuchen wir die Konvergenz des Schemas auf fünf unterschiedlichen Gittertypen. Wir erhalten ein Verfahren, das zweiter Ordnung genau ist für äquidistante und nicht äquidistante glatte Gitter, während es für lokal äquidistante Gitter nur eine Genauigkeit erster Ordnung liefert. Dabei tritt das unerwünschte Resultat auf, dass das Schema für oszillierende oder zufällige Gitter gar nicht konvergiert. Schliesslich testen wir die mathematischen Resultate anhand einiger numerischer Simulationen.

Die “fixed pivot”-Technik gibt eine konsistente Überschätzung der Lösung bei grossen Partikeln, wenn sie auf groben Gittern angewendet wird. Um dieses Problem zu bewältigen, wurde die Technik der Zellmittelung eingeführt, die alle Vorteile der “fixed pivot”-Technik enthält, aber die numerischen Ergebnisse verbessert. In der Arbeit haben wir dazu einige numerische Experimente durchgeführt. Die gewonnenen Resultate haben wir mit den Resultaten der 'fixed Pivot technik' verglichen. Diese Zellteilungsmethode liefert Konvergenz zweiter Ordnung auf gleichmässigen, ungleichmässigen aber glatten und lokal gleichmässigen Gittern. Nimmt man oszillierende oder zufällige Gitter, konvergiert die Methode nur mit erster Ordnung. Das heisst die Technik der Zellmittelung hat höhere Konvergenzordnung als die Fix pivot Technik für gleichmässigen, ungleichmässigen aber glatten und lokal gleichmässigen Gitter. Der mathematische Beweis der höheren Ordnung ist ein offenes Problem.

Contents

Chapter 1

Introduction

1.1 Overview

The continuous coagulation-fragmentation equations are a type of partial integro-differential equations which are also known as aggregation-breakage equations. These models describe the dynamics of particle growth and the time evolution of a system of particles under the combined effect of aggregation (or coagulation) and breakage (or fragmentation). Each particle is identified by its size (or volume) which is assumed to be a positive real number. From a physical point of view the basic mechanisms taken into account are the coalescence of two particles to form a larger one and the breakage of particles into smaller ones. These models are of substantial interest in many areas of science and engineering: kinetics of phase transformations in binary alloys such as segregation of binary alloys [62, 100], aggregation of red blood cells in biology [76], fluidized bed granulation processes [75, 74, 49], aerosol physics, i.e. the evolution of a system of solid or liquid particles suspended in a gas [83, 17, 85], formation of planets in astrophysics [79], polymer science [101] and many more.

In 1917, Smoluchowski proposed [87] the following discrete model in order to describe the coagulation of colloids moving according to a Brownian motion which is known as *Smoluchowski coagulation equation*

$$\frac{d}{dt}c_i = \frac{1}{2}\sum_{j=1}^{i-1} K_{j,i-j}c_jc_{i-j} - \sum_{j=1}^{\infty} K_{i,j}c_ic_j,$$

with

$$c_i(0) = c_i^0, \quad \text{for} \quad i = 1, 2, 3, \ldots.$$

Here the number density (or concentration) of particles of size i at time t is denoted by $c_i(t)$. The coagulation rates $K_{i,j}$ are non-negative real numbers such that $K_{i,j} = K_{j,i}$ for $i, j \geq 1$. The first term on the right-hand side in the above equation gives the birth of i-particles by coagulation of smaller particles while the second represents the death of

i-particles due to the coalescence with other particles. The factor $\frac{1}{2}$ will come to avoid the double counting in the birth term.

In 1928, Müller [71] provided the continuous version of the Smoluchowski coagulation equation as

$$\frac{\partial f(x,t)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)f(x-y,t)f(y,t)dy - \int_0^\infty K(x,y)f(x,t)f(y,t)dy,$$

with

$$f(x,0) = f_0(x).$$

Here the variables $x \geq 0$ and $t \geq 0$ denote the size of the particles and time, respectively. The number density of particles of size x at time t is denoted by $f(x,t)$. The coagulation kernel $K(x,y) \geq 0$ represents the rate at which the particles of size x coalesce with particles of size y and is assumed to be symmetric i.e. $K(x,y) = K(y,x)$.

The Smoluchowski coagulation equation only considers the coagulation process for the particles but does not include the fragmentation process. A straightforward generalization of the Smoluchowski equations are the *discrete coagulation-fragmentation equations* [88]. This is introduced as a model of an infinite system of ordinary differential equations which describes coagulation and binary fragmentation events together. The equations are as follows

$$\frac{d}{dt}c_i = \frac{1}{2}\sum_{j=1}^{i-1}(K_{i-j,j}c_{i-j}c_j - F_{i-j,j}c_j) - \sum_{j=1}^{\infty}(K_{i,j}c_ic_j - F_{i,j}c_{i+j}), \tag{1.1}$$

with

$$c_i(0) = c_i^0, \quad \text{for} \quad i = 1, 2, 3, \ldots.$$

Here $c = (c_i) \geq 0$ denotes the expected number of i-particle clusters per unit volume at time t. The coagulation rates $K_{i,j}$ and fragmentation rates $F_{i,j}$ are non-negative constants with $K_{i,j} = K_{j,i}$ and $F_{i,j} = F_{j,i}$.

In this thesis we deal with some issues related to the mathematical and numerical analysis of the continuous version of the coagulation-fragmentation equations, given by the following integral differential equations [89, 21]:

$$\begin{aligned}\frac{\partial f(x,t)}{\partial t} =& \frac{1}{2}\int_0^x K(x-y,y)f(x-y,t)f(y,t)dy - \int_0^\infty K(x,y)f(x,t)f(y,t)dy \\ &- \frac{1}{2}\int_0^x F(x-y,y)f(x,t)dy + \int_0^\infty F(x,y)f(x+y,t)dy,\end{aligned} \tag{1.2}$$

with

$$f(x,0) = f_0(x) \geq 0 \;\; a.e.$$

Note that this system is the continuous coagulation equation with binary fragmentation. Here the function $f(x,t)$ with the variables $x,\ t \geq 0$ and the coagulation kernel $K(x,y) \geq 0$ have the same interpretation as are in the case of continuous Smoluchowski coagulation equation. Here $f(x,t)dx$ represents the average number of particles between the masses x and $x+dx$ at time t. This average and all other averages are referred to a unit volume. The coagulation kernel $K(x,y)$ is introduced through the assumption that the number of coalescence between particles of mass $]x, x+dx[$ and those of mass $]y, y+dy[$ is $K(x,y)f(x,t)f(y,t)dxdydt$ during the time interval $]t, t+dt[$. In the same way, the fragmentation kernel $F(x,y) \geq 0$ gives the rate at which the particles of size $x+y$ break up into two particles of sizes x and y and is assumed to be symmetric i.e. $F(x,y) = F(y,x)$.

The integrals on the right-hand side of (1.2) represent, respectively,

- birth of particles of size x by the aggregation of particles with sizes y and $x-y$ $(0 \leq y \leq x)$
- death of particles of size x due to the aggregation with particles of size y $(0 \leq y < \infty)$
- death of particles of size x due to their breakage into particles of size y $(0 \leq y \leq x)$
- birth of particles of size x by the breakage of particles of size $x+y$ $(0 \leq y < \infty)$.

Actually, we will work with a more general form that allows multiple fragmentation where a particle may break into more than two fragments. A more general form of the above equation is given by Melzak [70] as the coagulation and multiple fragmentation equation. For the moment let us consider only the multiple-fragmentation process as

$$\frac{\partial f(x,t)}{\partial t} = \int_x^{\infty} \Gamma(y,x)f(y,t)dy - \int_0^x \frac{y}{x}\Gamma(x,y)f(x,t)dy, \tag{1.3}$$

with

$$f(x,0) = f_0(x) \geq 0 \;\; a.e.$$

where $\Gamma(x,y) \geq 0$ is the multiple-fragmentation kernel. The fragmentation kernel $\Gamma(x,y)$ enters by assuming that $f(x,t)\Gamma(x,y)dxdydt$ is the average number of particles of mass $]y, y+dy[$ obtained from the breakage of the particles of mass $]x, x+dx[$ during the time interval $]t, t+dt[$. Conservation of mass implies that $\partial f(x,t)/\partial t$ is equal to a sum of two terms which represent, respectively, the rates of

- birth of particles of size x by the breakage of particles of size y $(x \leq y < \infty)$,
- death of particles of size x due to their breakage into particles of size y $(0 \leq y \leq x)$.

Now the continuous coagulation and multiple fragmentation equation can also be written in the following form [56, 40]

$$\begin{aligned}\frac{\partial f(x,t)}{\partial t} =& \frac{1}{2}\int_0^x K(x-y,y)f(x-y,t)f(y,t)dy - \int_0^\infty K(x,y)f(x,t)f(y,t)dy \\ &+ \int_x^\infty b(x,y)S(y)f(y,t)dy - S(x)f(x,t),\end{aligned} \tag{1.4}$$

with

$$f(x,0) = f_0(x) \geq 0 \;\; a.e. \tag{1.5}$$

Here the breakage function $b(x,y)$ is the probability density function for the formation of particles of size x from the particles of size y. It is non-zero only for $x < y$. The selection function $S(x)$ describes the rate at which particles of size x are selected to break. The selection function S and breakage function b are defined in terms of the multiple-fragmentation kernel Γ used in (1.3) as

$$S(x) = \int_0^x \frac{y}{x}\Gamma(x,y)dy, \qquad b(x,y) = \Gamma(y,x)/S(y).$$

Equation (1.4) is usually referred as the generalized coagulation-fragmentation equation, as fragmenting particles can split into more than two pieces. However, the continuous coagulation and binary-fragmentation equation (1.2) can be obtained as a special case of (1.4) by setting

$$S(x) = \frac{1}{2}\int_0^x F(y,x-y)dy, \qquad b(x,y) = F(x,y-x)/S(y)$$

where F is assumed to be symmetric. In this binary-fragmentation model, the function $F(x-y,y)$ represents the rate at which particles of size $x-y$ and y are produced from a fragmenting particle of size x.

Before proceeding to the next section, it is important to define the moments of the number density distribution. The rth moment of the number density distribution $f(x,t)$ if it exists is defined by

$$M_r(t) = M_r(f(t)) := \int_0^\infty x^r f(x,t)dx, \quad r \in \mathbb{R}_{\geq 0}.$$

The first two moments represent some important properties of the distribution. The zeroth ($r = 0$) and first ($r = 1$) moments give the total number and the total mass or volume of particles, respectively.

1.2 Existing and new results

This work includes typical questions of mathematical and numerical analysis for the continuous coagulation-fragmentation equations. In particular, we deal mainly with the problem of existence and uniqueness of solutions for these equations. Moreover, the convergence analysis of sectional methods is also studied for non-linear coagulation problems. Now we start to give a short description to each of the topic mentioned above.

1.2.1 Existence of solutions

In the study of any equation, one of the first mathematical questions is: *Does the solution exist*? Many results on existence of solutions to the various forms of the coagulation-fragmentation equation have already been established using a number of different methods. A precise review of existing literature gives an idea on the conditions which are required to show the well-posedness of the coagulation-fragmentation equation. These conditions include some bounds on the kernels as well as the finiteness of total number of particles $\int_0^\infty f_0(x)dx$ and total mass $\int_0^\infty xf_0(x)dx$ taken initially.

Melzak and McLeod first discussed the existence of solutions in [70, 67, 68, 69]. Galkin, Dubovkskii and Stewart extended their result in [36, 21] using compactness methods in the space of continuous functions. Ball, Carr, Penrose, Spouge and Da Costa studied the discrete system of equations [5, 4, 88, 14] and Stewart, Escobedo, Laurençot, Mischler and Perthame [89, 27, 28, 57, 60] treated the continuous equations using compactness methods in the space of integrable functions. However, the case of multiple-fragmentation is not discussed too much. The first study of the coagulation equation with multiple fragmentation is due to Melzak [70] where the first existence result was proved for bounded coefficients. McLaughlin et al. [65] established the existence of solutions to the multiple-fragmentation equation under the condition that

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

where the sequence C_n may be unbounded. This was extended in McLaughlin et al. [66] to the combined coagulation and multiple-fragmentation equation (1.4) under the assumptions that K is constant and

$$\Gamma \in L^\infty(]0,\infty[\times]0,\infty[).$$

Using similar arguments, Lamb [56] discussed the existence of solutions to (1.4) under the less restrictive conditions that K is bounded, S satisfies a linear growth condition, and $b(x,y)$ is such that the break-up of a particle of size y is a mass-conserving process that produces an average number of smaller particles that is finite and independent of y. But most of them used one particular method that involves the application of the theory of semigroup of operators.

We prove the existence of solutions to (1.4). The proof is based on weak L^1 compactness methods applied to suitably chosen approximating equations. This approach originated in the work of Stewart [89] who investigated the case when both the coagulation kernel K and binary-fragmentation kernel F satisfy growth conditions almost up to linearity. Existence results for the continuous coagulation equation with multiple fragmentation were also established by Laurençot [57] with the approach of Stewart, the class of kernels being different but with a non-empty intersection. He considered only those coagulation kernels which have a product kernel as dominating part, see (B.19) in Appendix. But this is not the case for the class of coagulation kernels for which we prove the existence of solutions. We will also give some examples of coagulation kernels in Chapter 2 which satisfy our hypotheses but are not included in Laurençot [57]. A more complete result is available for the discrete coagulation equation with multiple fragmentation in Laurençot [58].

Here, our aim in Chapter 2 is to prove the existence of solutions to (1.4) under the much less restrictive conditions that K is unbounded and satisfies a certain growth condition as well as that S satisfies an almost linear growth condition. The present work improves the results of McLaughlin et al. [66] and Lamb [56] by relaxing the assumption of boundedness of the coagulation coefficient, the latter condition being crucial for the use of the semigroup approach.

In Chapter 2, we missed some classical fragmentation kernels which are of substantial interest in the engineering literature. Examples of these type of kernels are given in Chapter 2 which give the motivation for Chapter 4. The purpose of Chapter 4 is to extend the previous existence result discussed in Chapter 2. Here we will prove the existence of solutions to (1.4) under the same classes of coagulation kernels but more relaxed conditions on multiple fragmentation kernels. This result includes those classical kernels which are mentioned above.

1.2.2 Uniqueness

The next question in the study of any equation is the uniqueness of solutions if they exist. This has also been discussed by many researchers for the coagulation-fragmentation equations. Mathematical results on the issue have been derived by Aizenman and Bak [1] for constant kernels and by Melzak [70] for particular class of bounded kernels. Various existence and uniqueness results for unbounded coagulation kernels in the absence of fragmentation, have been established by Burobin [8], Burobin and Galkin [9], Ernst et al. [26], Galkin [35], Galkin and Dubovskii [36], McLeod [67]. Ziff and McGrady [103] have demonstrated existence for certain explicit bounded and unbounded fragmentation kernels. After this, Ball and Carr [4] considered the discrete coagulation-fragmentation equations whereas Stewart [89, 90, 91], Dubovskii and Stewart [21] have proved the existence, mass conservation and uniqueness with unbounded kernels for the continuous

equations. They considered linear growth on coagulation kernels with different classes of fragmentation kernels. Laurençot [60] has extended the existence results up to the bilinear growth, i.e. $k(1+x)(1+y)$, of the kernels with some additional restrictions at infinity. Escobedo et al. [29] have proved the uniqueness of self similar solutions only for the fragmentation equation. But they required some regularity of solutions to prove the uniqueness. Benjamin [6] has also investigated the uniqueness via a probabilistic interpretation for the discrete coagulation-fragmentation equation.
It has been proved by McLeod [67, 69] that for the unbounded multiplicative coagulation kernel $K = xy$ in absence of fragmentation, the mass conservation law for solutions breaks down at a finite time t_c, i.e.

$$\int_0^\infty xf(x,t)dx \neq \int_0^\infty xf_0(x)dx \quad \text{for all time} \quad t > t_c,$$

when the second moment blows-up. This phenomenon is known as *gelation* and is related to a *phase transition.* Ball and Carr [4] as well as Stewart [91] have shown the mass conservation when the coagulation kernels grow at most up to linearity. When the coagulation kernels lie between linear and bilinear growth, the existence and uniqueness of mass conserving solutions for discrete equations under strong fragmentation have been proven by Da Costa [14]. He noticed that a sufficiently strong fragmentation prevents the occurrence of the gelation phenomenon. Escobedo et al. [27] have also obtained the existence of at least one mass conserving solution with the same assumption on coagulation kernels with strong fragmentation for continuous equations. But the uniqueness was left as an open problem in this case. So the first objective of the Chapter 3 is to address this issue for coagulation equation with binary fragmentation (1.2). In this case, we make some additional restrictions on the fragmentation kernels to prove the uniqueness of mass conserving solutions. It should be pointed out that Laurençot and Mischler [59] also demonstrated the uniqueness for continuous equation in the class $\mathcal{C}([0,T], L^1_\phi(\mathbb{R}_{>0})) \bigcap L^1(0,T; L^1_{\phi^2}(\mathbb{R}_{>0}))$ for each $T > 0$. Here $L^1_\phi(\mathbb{R}_{>0})$ is denoted as the space of functions f such that $f\phi \in L^1(\mathbb{R}_{>0})$. They considered the following conditions on the kernels to investigate the uniqueness of solutions:

$$K(x,y) \leq \phi(x)\phi(y), \tag{1.6}$$

and

$$\int_0^x F(x-y,y)(\phi(y)+\phi(x-y)-\phi(x))dy \leq B\phi(x) \tag{1.7}$$

where ϕ is a subadditive function i.e., $\phi(x+y) \leq \phi(x)+\phi(y)$. In this case, the space considered by Laurençot and Mischler becomes more restrictive than $\mathcal{C}(\mathbb{R}_{\geq 0}, L^1(\mathbb{R}_{>0}))$, which was used in Escobedo et al. [27]. This is due to the assumption of the finiteness of higher moments of f by taking $L^1(0,T; L^1_{\phi^2}(\mathbb{R}_{>0}))$. So, due to the restrictiveness of the above space, it makes sense to demonstrate the uniqueness again in the larger space $\mathcal{C}(\mathbb{R}_{\geq 0}, L^1(\mathbb{R}_{>0}))$. Here we will prove the finiteness of these higher moments by using the strong fragmentation condition.

The second task in Chapter 3 is to consider the question of uniqueness of solutions to the continuous coagulation and multiple fragmentation equation (1.4) where we have the existence of solutions from Chapter 2. Here we prove the uniqueness of solutions with some additional restrictions on the coagulation and fragmentation kernels.

1.2.3 Convergence analysis

The coagulation-fragmentation equations can be solved analytically only for some specific examples of kernels, see [20, 33, 34]. In general we need to solve them numerically. Many numerical methods have been proposed to solve these equations: finite element methods [30, 72, 78], finite volume methods [7, 31, 32], stochastic methods [24, 25, 61], moment methods [94] and sectional methods [48, 50, 54, 55].

A large variety of finite element methods, finite volume methods, weighted residuals, the method of orthogonal collocation and Galerkin's method are implemented for solving these equations. By using these methods, we may have a good prediction of number density but a poor prediction of moments, see J. Kumar et al. [53]. These methods are computationally very expensive and include stability problems. In moment methods, these equations are transformed into a system of ordinary differential equations describing the evolution of the moments of the particle size distribution or number density distribution. The moment methods indeed predict very accurately the moments of the distribution but are unable to give precise information about the density distribution. In recent times, the *sectional methods* have become computationally very attractive because they not only predict accurately some selected moments of the distribution, but also give satisfactory results for the complete density distribution.

Several authors have proposed sectional methods for these equations: S. Kumar and Ramkrishna [54, 55], J. Kumar et al. [48, 50] and Vanni [97]. Among all sectional methods, the *fixed pivot technique* given by S. Kumar and Ramkrishna [54] is the most extensively used method these days due to its generality and robustness. This technique also efficiently works for a multi-dimensional size variable [13]. It predicts the first two moments of the distribution very accurately. Despite the fact that the first two numerically calculated moments are fairly accurate, the fixed pivot technique consistently over-predicts the results of number density as well as its higher moments in the large size range when applied on coarse grids [47]. A step to improve the fixed pivot technique by preserving all advantages of the existing sectional methods has been recently made by J. Kumar et al. [48, 50] as the *cell average technique.*

Recently J. Kumar and Warnecke [51, 52] have published the numerical analysis of sectional methods for pure breakage or fragmentation problems. This case was simpler due to the linearity of that equation. But the convergence analysis of these methods was still open for pure aggregation or coagulation problems. This is a challenging task due to the non-linearity of the equation. The purpose of the Chapters 5 is to demonstrate the missing numerical analysis of the most popular *fixed pivot method* among all sectional methods for nonlinear aggregation problems. In this chapter, we discuss the convergence analysis of the *fixed pivot method* for these equations and verify the mathematical results by several numerical simulations. The aim of Chapter 6 is to compute the order of convergence of the *cell average technique* for the same problem by taking a few numerical examples. Finally, the numerical results obtained are also compared with those of the fixed pivot technique which improve the order of convergence on coarse grids. The mathematical analysis of the *cell average technique* for aggregation problems is still an open problem.

1.3 Outline of thesis

Let us now briefly outline the content of the thesis as follows:

In Chapter 2 we state and prove an existence theorem for the coagulation and multiple fragmentation equation (1.4) with unbounded kernels. This existence proof is motivated by the approach developed by Stewart [89] for the coagulation equation with binary fragmentation which was based on the weak L^1 compactness methods. This approach is also well-suited when the multiple fragmentation is taken into account with coagulation equation.

Chapter 3 deals with two different uniqueness results for coagulation-fragmentation equations. In the first result, we study the uniqueness of mass conserving solutions for coagulation and binary fragmentation equation (1.2) under strong fragmentation. The existence of mass conserving solutions is followed from Escobedo et al. [27]. The second result focuses on the uniqueness of solutions for coagulation equation with multiple fragmentation (1.4) where Chapter 2 supports the existence of solutions.

Further, we prove a new result on existence of solutions to the continuous coagulation equation with multiple fragmentation (1.4). The result is an extension of the previous result in Chapter 2. The existence of solutions is achieved under much less restrictive conditions on multiple fragmentation kernels.

We then proceed to introduce the convergence analysis of the fixed pivot technique [54] for solving the pure nonlinear coagulation equations in Chapter 5. The order of convergence is investigated on five different kind of uniform and non-uniform meshes, together with some numerical examples that back up the validity of the mathematical observations.

The fixed pivot technique discussed in Chapter 5 yields a consistent over-prediction of number density for the large size particles on coarse grids. This gives us a diverging behavior of higher moments. Therefore, the cell average technique came into the picture to improve the numerical results. In Chapter 6 we calculate the order of convergence of the cell average technique to the pure coagulation problems numerically and the numerical results obtained are also compared with the results for the case of the fixed pivot technique.

Chapter 7 presents some general conclusions regarding this work and some open problems for the future developments.

At the end, some appendices are also given which play an important role in the construction of this thesis.

Chapter 2 and the second part of Chapter 3 is published in the Journal of Mathematical Analysis and Applications [40]. The first part of Chapters 3 is under review in [39]. The Chapters 4, 5 and 6 will be submitted for publications, see [41, 38, 37] respectively.

Chapter 2

Existence of solutions

This chapter deals with our main result on existence of solutions to the continuous coagulation equation with multiple fragmentation whenever the kernels satisfy certain growth conditions. The proof relies on weak L^1 compactness methods applied to suitably chosen approximating equations. Solutions are shown to be in the space

$$X^+ = \left\{ f \in L^1 : \int_0^\infty (1+x)|f(x)|dx < \infty, f \geq 0 \;\; a.e. \right\}$$

for non-negative initial data $f_0 \in X^+$. The result is an extension of previous results of Lamb [56] that covers some kernels modeling particles in flows that were not included in the previous results. The main novelty of the result is that it includes *multiple fragmentation.*

The chapter is organized as follows. In Section 2.1, we repeat a brief description of equation from Chapter 1 and give some definitions and hypotheses which are required to study the subsequent sections. In Section 2.2, we extract a weakly convergent subsequence in L^1 from a sequence of unique solutions for truncated equations to (2.1)-(2.2). Then we prove in Theorem 2.2.3 that the limit function obtained from weakly convergent subsequence is indeed a solution to (2.1)-(2.2).

2.1 Introduction

Let us recall nonlinear continuous coagulation and multiple fragmentation equation from chapter 1:

$$\begin{aligned}\frac{\partial f(x,t)}{\partial t} =& \frac{1}{2}\int_0^x K(x-y,y)f(x-y,t)f(y,t)dy - \int_0^\infty K(x,y)f(x,t)f(y,t)dy \\ &+ \int_x^\infty b(x,y)S(y)f(y,t)dy - S(x)f(x,t), \qquad (2.1)\end{aligned}$$

with

$$f(x,0) = f_0(x) \geq 0 \;\; a.e. \tag{2.2}$$

Here the variables $x \geq 0$ and $t \geq 0$ denote the size of the particles and time, respectively. The number density of particles of size x at time t is denoted by $f(x,t)$. The coagulation kernel $K(x,y)$ represents the rate at which particles of size x coalesce with particles of size y. The fragmentation terms have a similar interpretation. The breakage function $b(x,y)$ is the probability density function for the formation of particles of size x from the particles of size y. It is non-zero only for $x < y$. The selection function $S(x)$ describes the rate at which particles of size x are selected to break. The selection function S and breakage function b are defined in terms of the multiple-fragmentation kernel Γ as

$$S(x) = \int_0^x \frac{y}{x}\Gamma(x,y)dy, \qquad b(x,y) = \Gamma(y,x)/S(y). \tag{2.3}$$

The breakage function has the following properties

$$\int_0^y b(x,y)dx = N < \infty, \;\; \text{for all} \;\; y > 0 \;\; \text{and} \quad b(x,y) = 0, \;\; \text{for} \;\; x > y, \tag{2.4}$$

and

$$\int_0^y xb(x,y)dx = y \;\; \text{for all} \;\; y > 0. \tag{2.5}$$

The quantity N represents the number of fragments obtained from the breakage of particles of size y. In this work, we assume that this quantity is size independent, a more general case is not treated here is to let N be a function of y. For the total mass in the system to remain conserved during fragmentation events, b must satisfy the equation (2.5). It states that the total mass of the fragments equals the original mass when a particle of mass y breaks.

Let X be the following Banach space with norm $\|\cdot\|$

$$X = \{f \in L^1(0,\infty) : \|f\| < \infty\} \;\; \text{where} \;\; \|f\| = \int_0^\infty (1+x)|f(x)|dx.$$

We also write

$$\|f\|_x = \int_0^\infty x|f(x)|dx \;\; \text{and} \;\; \|f\|_1 = \int_0^\infty |f(x)|dx$$

and set

$$X^+ = \{f \in X : f \geq 0 \;\; a.e.\}.$$

Hypotheses 2.1.1. *(H1) K is a continuous non-negative function on $[0,\infty[\times[0,\infty[$ and Γ is a non-negative locally bounded function,*

(H2) K is symmetric, i.e. $K(x,y) = K(y,x)$ for all $x, y \in]0,\infty[$,

(H3) $K(x,y) \le \phi(x)\phi(y)$ for all $x, y \in]0,\infty[$ where $\phi(x) \le k_1(1+x)^{\mu}$ for some $0 \le \mu < 1$ and constant k_1.

(H4) $S :]0,\infty[\mapsto [0,\infty[$ is continuous and satisfies the bound $S(x) \le k_2(1+x)^{\gamma}$ for all $x \in]0,\infty[$ where $0 \le \gamma < 1$ and k_2 is a constant.

Definition 2.1.2. *Let $T \in]0,\infty]$. A solution f of (2.1-2.2) is a function $f : [0,T[\to X^+$ such that for a.e. $x \in]0,\infty[$ and all $t \in [0,T[$ the following hold*

(i) $f(x,t) \ge 0$,

(ii) $f(x,.)$ is continuous on $[0,T[$,

(iii) the following integrals are bounded

$$\int_0^t \int_0^\infty K(x,y) f(y,s)dyds < \infty \quad \text{and} \quad \int_0^t \int_x^\infty b(x,y)S(y)f(y,s)dyds < \infty,$$

(iv) the function f satisfies the following weak formulation of (2.1)

$$\begin{aligned} f(x,t) = f_0(x) + \int_0^t \bigg\{ \frac{1}{2}\int_0^x & K(x-y,y)f(x-y,s)f(y,s)dy \\ - \int_0^\infty K(x,y)f(x,s)f(y,s)dy &+ \int_x^\infty b(x,y)S(y)f(y,s)dy - S(x)f(x,s) \bigg\} ds. \end{aligned}$$

For the completeness of the Definition 2.1.2 of solutions to (2.1), we give the following lemma

Lemma 2.1.3. *For any $f \in X^+$, the integrals in Definition 2.1.2 (iv) exist for a.e. $x \in]0,\infty[$ under Hypotheses 2.1.1.*

Proof. We consider the following integral, by changing the order of integration and substituting $x - y = x'$, $y = y'$ and (H3)

$$\begin{aligned} \int_0^\infty \int_0^x K(x-y,y)f(x-y,s)f(y,s)dydx &= \int_0^\infty \int_0^\infty K(x,y)f(x,s)f(y,s)dxdy \\ &\le k_1^2 \int_0^\infty \int_0^\infty (1+x)^{\mu}(1+y)^{\mu} f(x,s)f(y,s)dxdy \\ &< \infty. \end{aligned}$$

Thus, by applying Fubini's Theorem [42, 21.13], we obtain

$$\int_0^x K(x-y,y)f(x-y,s)f(y,s)dy \ \text{ and } \ \int_0^\infty K(x,y)f(x,s)f(y,s)dy$$

exist for a.e. $x \in]0,\infty[$. Now for the following integral, by changing the order of integration, using(2.4) and (H4) we get

$$\begin{aligned}\int_0^\infty \int_x^\infty b(x,y)S(y)f(y,s)dydx &= \int_0^\infty \int_0^y b(x,y)S(y)f(y,s)dxdy \\ &= N\int_0^\infty S(y)f(y,s)dy \\ &\leq Nk_2 \int_0^\infty (1+y)^\gamma f(y,s)dy < \infty.\end{aligned}$$

Similarly, we find that

$$\int_x^\infty b(x,y)S(y)f(y,s)dy \ \text{ and } \ S(x)f(x,t)$$

exist for a.e. $x \in]0,\infty[$. □

We know a few specific coagulation kernels which satisfy the hypotheses mentioned above, see the Appendix B.5. However, they do not satisfy the assumptions of previously existing results on coagulation together with multiple fragmentation given in Lamb [56]. These kernels are the following:

(1) Shear kernel (non-linear velocity profile) Aldous [2] or Smit et al. [86] who use the length coordinate $\lambda = x^{\frac{1}{3}}$

$$K(x,y) = k_0(x^{1/3}+y^{1/3})^{7/3}.$$

(2) The modified Smoluchowski kernel, see Koch et al. [46], is given as

$$K(x,y) = k_0 \frac{(x^{1/3}+y^{1/3})^2}{x^{1/3}\cdot y^{1/3}+c}$$

with some fixed constant $c > 0$.

(3) Ding et al. [16] used the following kernel in the application of population balance models to activated sludge flocculation

$$K(x,y) = k_0 \frac{(x^{1/3}+y^{1/3})^q}{1+\left(\frac{x^{1/3}+y^{1/3}}{2y_c^{1/3}}\right)^3}, \qquad 0 \leq q < 3.$$

Here q is the order of the kernel.

Further we point out that the modified Smoluchowski kernel was derived from the Smoluchowski kernel or Brownian motion kernel given as, see Aldous [2] or Smit et al. [86],

$$K(x,y) = k_0(x^{1/3} + y^{1/3})(x^{-1/3} + y^{-1/3})$$

which can be rewritten as

$$K(x,y) = k_0 \frac{(x^{1/3} + y^{1/3})^2}{x^{1/3} \cdot y^{1/3}}.$$

The modification eliminates the singular behavior of this kernel. The original Smoluchowski kernel does not satisfy (H3) in contrast to the modified one by Koch et al. [46].

Now we take the following type of fragmentation kernels which also satisfy the hypotheses mentioned above

$$S(x) = x^{\sigma}(1+x)^{\gamma-\sigma} \quad \text{and} \quad b(x,y) = \frac{\alpha+2}{y}\left(\frac{x}{y}\right)^{\alpha}, \quad 0 < x < y,$$

where $\sigma \geq 1 > \gamma \geq 0$ and $\alpha \geq 0$. This is the cut-off version of the classical selection functions $S(x) = x^{\gamma}$ which have been studied in Peterson [77] and also in Ziff [102]. If we write it rather as

$$S(x) = x^{\sigma}(\delta + x)^{\gamma-\sigma}.$$

In the limit $\delta \to 0$ one recovers the classical kernel.

2.2 Existence

2.2.1 The truncated problem

We prove the existence of solutions to (2.1-2.2) by taking the limit of a sequence of approximating equations obtained by replacing the kernel K and selection function S by the 'cut-off' kernels K_n and S_n, motivated by Stewart [89], where

$$K_n(x,y) := \begin{cases} K(x,y) & \text{if } x+y < n, \\ 0 & \text{if } x+y \geq n, \end{cases}$$

$$S_n(x) := \begin{cases} S(x) & \text{if } 0 < x < n, \\ 0 & \text{if } x \geq n. \end{cases}$$

The resulting equations, with solutions denoted by f^n, are written as

$$\begin{aligned}\frac{\partial f^n(x,t)}{\partial t} =& \frac{1}{2}\int_0^x K_n(x-y,y)f^n(x-y,t)f^n(y,t)dy - \int_0^{n-x} K_n(x,y)f^n(x,t)f^n(y,t)dy \\ &+ \int_x^n b(x,y)S_n(y)f^n(y,t)dy - S_n(x)f^n(x,t), \end{aligned} \tag{2.6}$$

with

$$f_0^n(x) := \begin{cases} f_0(x) & \text{if } 0 < x < n, \\ 0 & \text{if } x \geq n. \end{cases} \tag{2.7}$$

Choose $T > 0$. Proceeding as in [89, Theorem 3.1] we obtain the following result. For each $n = 1, 2, 3, \ldots$, (2.6-2.7) has a unique solution $f^n \in X^+$ with $f^n(x,t) \geq 0$ for a.e. $x \in]0, n[$ and $t \in [0, \infty[$, see Walker [98] also. Moreover, the total mass remains conserved, for all $t \in [0, \infty[$, i.e.

$$\int_0^n x f^n(x,t)dx = \int_0^n x f_0^n(x)dx. \tag{2.8}$$

From now on we consider the 'zero extension' of each f^n on $\mathbb{R}$, i.e.

$$\widehat{f^n}(x,t) := \begin{cases} f^n(x,t) & \text{if } 0 < x < n, \quad t \in [0,T] \\ 0 & \text{if } x \leq 0 \quad \textit{or} \quad x \geq n. \end{cases}$$

For the simplicity we drop the $\widehat{\cdot}$ notation for the remainder of the work and the suffixes on the coagulation kernels and the selection functions.

Next, we need to prove the following lemma to apply the *Dunford-Pettis-Theorem* [23, Theorem 4.21.2] and then equicontinuity of the sequence $(f^n)_{n\in\mathbb{N}}$ in time to use *Arzelà-Ascoli Theorem* [3, Appendix A8.5].

Lemma 2.2.1. *Assume that (H1), (H2), and (H4) hold. Then the following results are true:*

(i) $\displaystyle\int_0^\infty (1+x)f^n(x,t)dx \leq L$ *for* $n = 1, 2, 3\ldots$ *and all* $t \in [0,T]$,

(ii) given $\epsilon > 0$ *there exists an* $R > 0$ *such that for all* $t \in [0,T]$

$$\sup_n \left\{ \int_R^\infty f^n(x,t)dx \right\} \leq \epsilon,$$

(iii) given $\epsilon > 0$ there exists a $\delta > 0$ such that for all $n = 1, 2, 3\ldots$ and $t \in [0, T]$

$$\int_E f^n(x,t)dx < \epsilon \quad \textit{whenever} \quad \lambda(E) < \delta.$$

Proof. (i) From (2.6) and Fubini's Theorem, for each $n \geq 1$ we have by integration with respect to x and t

$$\begin{aligned}\int_0^1 f^n(x,t)dx =& -\frac{1}{2}\int_0^t\int_0^1\int_0^{1-x} K(x,y)f^n(x,s)f^n(y,s)dydxds\\ &-\int_0^t\int_0^1\int_{1-x}^{n-x} K(x,y)f^n(x,s)f^n(y,s)dydxds\\ &+\int_0^t\int_0^1\int_x^n b(x,y)S(y)f^n(y,s)dydxds - \int_0^t\int_0^1 S(x)f^n(x,s)dxds\\ &+\int_0^1 f^n(x,0)dx.\end{aligned}$$

Since the integrands are all non-negative, we may estimate

$$\begin{aligned}\int_0^1 f^n(x,t)dx \leq& \int_0^t\int_0^1\int_x^n b(x,y)S(y)f^n(y,s)dydxds + \int_0^1 f^n(x,0)dx\\ =& \int_0^t\int_0^1\int_x^1 b(x,y)S(y)f^n(y,s)dydxds\\ &+\int_0^t\int_0^1\int_1^n b(x,y)S(y)f^n(y,s)dydxds + \int_0^1 f^n(x,0)dx.\end{aligned}$$

Using Fubini's Theorem, (H4) and (2.4) in the size independent case, we obtain

$$\begin{aligned}\int_0^1 f^n(x,t)dx \leq& \int_0^t\int_0^1\int_0^y b(x,y)S(y)f^n(y,s)dxdyds\\ &+\int_0^t\int_1^n\int_0^1 b(x,y)S(y)f^n(y,s)dxdyds + \int_0^1 f^n(x,0)dx\\ \leq& k_2N\int_0^t\int_0^1(1+y)^\gamma f^n(y,s)dyds + k_2N\int_0^t\int_1^n(1+y)^\gamma f^n(y,s)dyds\\ &+\int_0^1 f^n(x,0)dx\\ \leq& k_2N\int_0^t\int_0^1(1+y)f^n(y,s)dyds + 2k_2N\int_0^t\int_1^n yf^n(y,s)dyds\\ &+\int_0^1 f^n(x,0)dx. \qquad (2.9)\end{aligned}$$

From equation (2.8), for $s \in [0, T]$

$$\|f^n(s)\|_x = \|f^n(0)\|_x \leq \|f(0)\|. \tag{2.10}$$

Using (2.9) and (2.10) we obtain

$$\begin{aligned}\int_0^1 f^n(x,t)dx &\leq k_2 N \int_0^t \int_0^1 f^n(y,s)dyds + 3k_2NT\|f_0\| + \|f_0\| \\ &= k_2 N \int_0^t \int_0^1 f^n(y,s)dyds + \|f_0\|\{3k_2NT + 1\}.\end{aligned}$$

Applying Gronwall's Lemma, see e.g. Walter [99, p. 310], we obtain

$$\int_0^1 f^n(x,t)dx \leq \|f_0\|\{3k_2NT + 1\}\exp\{k_2NT\}.$$

Thus, by using (2.8) again we may estimate

$$\begin{aligned}\int_0^\infty (1+x)f^n(x,t)dx &= \int_0^1 f^n(x,t)dx + \int_1^n f^n(x,t)dx + \int_0^n xf^n(x,t)dx \\ &\leq \int_0^1 f^n(x,t)dx + \int_1^n xf^n(x,t)dx + \|f_0\| \\ &\leq \|f_0\|\{(3k_2NT+1)\exp(k_2NT) + 2\} := L.\end{aligned}$$

(ii) For $\epsilon > 0$, let $R > 0$ be such that $R > \|f_0\|/\epsilon$. Then, by (2.10), for each $n = 1, 2, 3, \ldots$ and for all $t \in [0, T]$ we have

$$\begin{aligned}\int_R^\infty f^n(x,t)dx &= \int_R^\infty (x/x)f^n(x,t)dx \\ &\leq \frac{1}{R}\int_R^\infty xf^n(x,t)dx \leq \frac{1}{R}\|f_0\| < \epsilon.\end{aligned}$$

(iii) Choose $\epsilon > 0$ and let $E \subset \mathbb{R}_{>0} :=]0, \infty[$. By part (ii) we can choose $m > 1$ such that for all $n = 1, 2, 3, \ldots$ and $t \in [0, T]$

$$\int_m^\infty f^n(x,t)dx < \epsilon/2. \tag{2.11}$$

Let χ denotes the characteristic function, i.e.

$$\chi_E(x) := \begin{cases} 1 & \text{if } x \in E, \\ 0 & \text{if } x \notin E, \end{cases}$$

and for $n = 1, 2, 3, \ldots$ and $t \in [0, T]$, define

$$p^n(E,t) = \sup_{0 \leq z \leq m} \int_{\mathbb{R}_{>0}} \chi_{E \bigcap]0,m]}(x+z)f^n(x,t)dx.$$

Set

$$K_0 = \sup_{\substack{0\le x\le m\\ 0\le y\le m}} \frac{1}{2} K(x,y) \quad \text{and} \quad F_0 = \sup_{\substack{0\le y\le r\\ 0\le x\le m}} \Gamma(y,x). \tag{2.12}$$

Consider $\gamma \in [0,1[$ and k_2 as in (H4), N as given by (2.4). Then one can choose $r > m$ such that

$$k_2 NTL(1+r)^{\gamma-1} < \epsilon/\{8\exp(TLK_0)\}. \tag{2.13}$$

By the absolute continuity of integral, there exists a $\delta_1 > 0$ such that

$$p^n(E,0) \le \sup_{0\le z\le m} \int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+z) f_0(x)dx < \epsilon/\{4\exp(TLK_0)\} \tag{2.14}$$

for all n whenever $\lambda(E) \le \delta_1$ for the Lebesgue measure λ. Also, there exists a $\delta_2 > 0$ such that

$$\sup_{0\le z\le m} \int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+z)dx < \epsilon/\{8TF_0L\exp(TLK_0)\} \tag{2.15}$$

whenever $\lambda(E) \le \delta_2$. Set $\delta = \min\{\delta_1, \delta_2\}$. Using the non-negativity of each f^n we can use (2.6-2.7) to prove that for $0 < z < m$ and $\lambda(E) < \delta$

$$\begin{aligned}
&\int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+z) f^n(x,t)dx \\
&\quad \le \frac{1}{2}\int_0^t \int_{\mathbb{R}_{>0}} \int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+z)\chi_{]0,x]\bigcap]0,m]}(y) K(x-y,y) f^n(x-y,s) f^n(y,s)dydxds \\
&\quad\quad + \int_0^t \int_0^m \chi_{E\bigcap]0,m]}(x+z) \int_x^n b(x,y)S(y)f^n(y,s)dydxds + p^n(E,0).
\end{aligned}$$

Using the substitution $x' = x-y$, $y' = y$ and Fubini's theorem in the first and second integrals on the right hand side respectively we find that

$$\begin{aligned}
&\int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+z) f^n(x,t)dx \\
&\quad \le \frac{1}{2}\int_0^t \int_{\mathbb{R}_{>0}} \int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+y+z)\chi_{]0,m]}(y) K(x,y) f^n(x,s) f^n(y,s)dydxds \\
&\quad\quad + \int_0^t \int_0^m \int_0^y \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y)f^n(y,s)dxdyds \\
&\quad\quad + \int_0^t \int_m^n \int_0^m \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y)f^n(y,s)dxdyds + p^n(E,0).
\end{aligned}$$

By the definition of $p^n(E,t)$, (2.12) and Lemma 2.2.1(i), this can be rewritten as

$$\begin{aligned}
&\int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+z) f^n(x,t)dx \\
\leq & K_0 \int_0^t \int_0^m f^n(y,s) \sup_{0\leq v\leq m} \int_{\mathbb{R}_{>0}} \chi_{E\bigcap]0,m]}(x+v) f^n(x,s)dxdyds \\
&+ \int_0^t \int_0^m \int_0^m \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y) f^n(y,s)dxdyds \\
&+ \int_0^t \int_m^r \int_0^m \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y) f^n(y,s)dxdyds \\
&+ \int_0^t \int_r^\infty \int_0^m \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y) f^n(y,s)dxdyds + p^n(E,0), \\
\leq & K_0 L \int_0^t p^n(E,s)ds + \int_0^t \int_0^r \int_0^m \chi_{E\bigcap]0,m]}(x+z)\Gamma(y,x) f^n(y,s)dxdyds \\
&+ \int_0^t \int_r^\infty \int_0^y \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y) f^n(y,s)dxdyds + p^n(E,0). \qquad (2.16)
\end{aligned}$$

We use (2.12), (2.15) and Lemma 2.2.1(i) to consider the following integral

$$\begin{aligned}
&\int_0^t \int_0^r \int_0^m \chi_{E\bigcap]0,m]}(x+z)\Gamma(y,x) f^n(y,s)dxdyds \\
&\qquad \leq F_0 \int_0^t \int_0^r f^n(y,s)dyds \cdot \epsilon/\{8TF_0L\exp(TLK_0)\} \\
&\qquad \leq \epsilon/\{8\exp(TLK_0)\}. \qquad (2.17)
\end{aligned}$$

By using (2.4), (H4), Lemma 2.2.1(i) and (2.13) we consider the following integral

$$\begin{aligned}
&\int_0^t \int_r^\infty \int_0^y \chi_{E\bigcap]0,m]}(x+z) b(x,y)S(y) f^n(y,s)dxdyds \\
&\qquad \leq k_2 N \int_0^t \int_r^\infty (1+y)^\gamma f^n(y,s)dyds \\
&\qquad \leq k_2 NTL(1+r)^{\gamma-1} < \epsilon/\{8\exp(TLK_0)\}. \qquad (2.18)
\end{aligned}$$

It can be deduced from (2.14), (2.16), (2.17) and (2.18) that

$$p^n(E,t) \leq K_0 L \int_0^t p^n(E,s)ds + \epsilon/\{2\exp(TLK_0)\}.$$

By using Gronwall's inequality, see e.g. Walter [99, p. 310], we obtain

$$p^n(E,t) \leq \exp(TLK_0)\epsilon/\{2\exp(TLK_0)\} = \epsilon/2. \qquad (2.19)$$

By (2.11) and (2.19), we obtain for $n = 1, 2, 3, \dots$ and $t \in [0, T]$

$$\begin{aligned}\int_E f^n(x,t)dx &= \int \chi_{E\bigcap]0,m]}(x) f^n(x,t)dx + \int \chi_{E\bigcap [m,\infty[}(x) f^n(x,t)dx \\ &\le p^n(E,t) + \int_m^\infty f^n(x,t)dx \\ &< \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon\end{aligned}$$

whenever $\lambda(E) < \delta$. □

The above Lemma 2.2.1 implies that for each $t \in [0, T]$, the sequence of functions $(f^n(t))_{n\in\mathbb{N}}$ lies in a weakly relatively compact set in $L^1]0, \infty[$ by the *Dunford-Pettis-Theorem.*

2.2.2 Equicontinuity in time

Now we proceed in this section to show equicontinuity of the sequence $(f^n)_{n\in\mathbb{N}}$ in time. It should be mentioned that (H3) is now assumed to be satisfied. Choose $\epsilon > 0$ and $\phi \in L^\infty]0, \infty[$. Let $s, t \in [0, T]$ and assume $t \ge s$. Choose $m > 1$ such that

$$\|\phi\|_{L^\infty} 2L/m < \epsilon/2. \tag{2.20}$$

For each n, by Lemma 2.2.1(i),

$$\int_m^\infty |f^n(x,t) - f^n(x,s)|dx \le \frac{1}{m}\int_m^\infty x\{f^n(x,t) + f^n(x,s)\}dx \le 2L/m. \tag{2.21}$$

By using (2.6), (2.20) and (2.21), we get using $t \ge s$

$$\begin{aligned}\Big|\int_0^\infty \phi(x)\{f^n(x,t) - f^n(x,s)\}dx\Big| \\ &\le \Big|\int_0^m \phi(x)\{f^n(x,t) - f^n(x,s)\}dx\Big| \\ &\quad + \int_m^\infty |\phi(x)|\{|f^n(x,t) - f^n(x,s)|\}dx \\ &\le \|\phi\|_{L^\infty} \int_s^t \Big[\frac{1}{2}\int_0^m \int_0^x K(x-y,y) f^n(x-y,\tau) f^n(y,\tau)dydx \\ &\quad + \int_0^m \int_0^{n-x} K(x,y) f^n(x,\tau) f^n(y,\tau)dydx \\ &\quad + \int_0^m \int_x^n b(x,y) S(y) f^n(y,\tau)dydx \\ &\quad + \int_0^m S(x) f^n(x,\tau)dx\Big] d\tau + \epsilon/2.\end{aligned} \tag{2.22}$$

Now we consider the first term on the right hand side of (2.22), by Fubini's Theorem, (H1)-(H4) and Lemma 2.2.1 (i)

$$
\begin{aligned}
&\frac{1}{2}\int_0^m \int_0^x K(x-y,y)f^n(x-y,\tau)f^n(y,\tau)dydx \\
&\qquad = \frac{1}{2}\int_0^m \int_y^m K(x-y,y)f^n(x-y,\tau)f^n(y,\tau)dxdy \\
&\qquad = \frac{1}{2}\int_0^m \int_0^{m-y} K(x,y)f^n(x,\tau)f^n(y,\tau)dxdy \\
&\qquad = \frac{1}{2}\int_0^m \int_0^{m-x} K(y,x)f^n(y,\tau)f^n(x,\tau)dydx \\
&\qquad = \frac{1}{2}\int_0^m \int_0^{m-x} K(x,y)f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \le k_1^2\frac{1}{2}\int_0^m \int_0^{m-x} (1+x)^\mu(1+y)^\mu f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \le \frac{1}{2}k_1^2L^2.
\end{aligned}
$$

For the second term we may estimate

$$
\begin{aligned}
&\int_0^m \int_0^{n-x} K(x,y)f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \le k_1^2\int_0^m \int_0^{n-x} (1+x)^\mu(1+y)^\mu f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \le k_1^2L^2.
\end{aligned}
$$

For $n > m$, the third term using (2.4) gives that

$$
\begin{aligned}
&\int_0^m \int_x^n b(x,y)S(y)f^n(y,\tau)dydx \\
&\qquad \le k_2\int_0^m \int_0^y b(x,y)(1+y)^\gamma f^n(y,\tau)dxdy \\
&\qquad\quad + k_2\int_m^n \int_0^m b(x,y)(1+y)^\gamma f^n(y,\tau)dxdy \\
&\qquad \le k_2 N\int_0^n (1+y)^\gamma f^n(y,\tau)dy \le k_2NL.
\end{aligned}
$$

Similarly we can obtain the above inequality for $m > n$.
For the fourth term we have

$$\int_0^m S(x)f^n(x,t)dx \le k_2L.$$

By using the above inequalities, the equation (2.22) reduces to

$$\left| \int_0^\infty \phi(x)\{f^n(x,t) - f^n(x,s)\}dx \right|$$
$$\leq \|\phi\|_{L^\infty]0,\infty[}(t-s)\left\{\frac{3}{2}k_1^2 L^2 + k_2(N+1)L\right\} + \epsilon/2 < \epsilon \qquad (2.23)$$

whenever $t - s < \delta$ for some $\delta > 0$. The argument given above similarly holds if $s > t$. Hence (2.23) is true for all n and $|t - s| < \delta$. This implies the time equicontinuity of the family $\{f^n(t), t \in [0,T]\}$ in $L^1(\mathbb{R}_{>0})$. Thus, $\{f^n(t), t \in [0,T]\}$ lies in a relatively compact subset of the *gauge space* Ω. The gauge space Ω is the space $L^1(\mathbb{R}_{>0})$ provided with a certain weak topology. Details concerning the gauge space can be found in Stewart [89]. So, we may apply refined version of *Arzelà-Ascoli Theorem*, see Stewart [89, Theorem 2.1] to conclude that there exists a subsequence f^{n_k} such that

$$f^{n_k}(t) \to f(t) \ \text{ in } \ \Omega \ \text{ as } \ n_k \to \infty$$

uniformly for $t \in [0,T]$ and for some $f \in C([0,T];\Omega)$.

2.2.3 Convergence of the approximations of the integrals

For simplicity of notation we mostly suppress the dependence on arbitrary but fixed $t \in [0,T]$ when it is not explicitly needed. Now we have to show that the limit function which we obtained above is indeed a solution to (2.1-2.2). Define the operators Q_i^n, Q_i, $i = 1$ to 4, to be

$$Q_1^n(f^n)(x) = \frac{1}{2}\int_0^x K(x-y,y)f^n(x-y)f^n(y)dy,$$
$$Q_1(f)(x) = \frac{1}{2}\int_0^x K(x-y,y)f(x-y)f(y)dy,$$
$$Q_2^n(f^n)(x) = \int_0^{n-x} K(x,y)f^n(x)f^n(y)dy, \qquad Q_2(f)(x) = \int_0^\infty K(x,y)f(x)f(y)dy,$$
$$Q_3^n(f^n)(x) = S(x)f^n(x), \qquad Q_3(f)(x) = S(x)f(x),$$
$$Q_4^n(f^n)(x) = \int_x^n b(x,y)S(y)f^n(y)dy, \qquad Q_4(f)(x) = \int_x^\infty b(x,y)S(y)f(y)dy,$$

where $f \in L^1]0,\infty[$, $x \in]0,\infty[$ and $n = 1,2,3,\ldots$. Set $Q^n = Q_1^n - Q_2^n - Q_3^n + Q_4^n$ and $Q = Q_1 - Q_2 - Q_3 + Q_4$.

Lemma 2.2.2. *Suppose $(f^n)_{n\in\mathbb{N}} \subset X^+$, $f \in X^+$, where $||f^n|| \leq L$, and $f^n \rightharpoonup f$ in $L^1]0,\infty[$ as $n \to \infty$. Then for each $m > 0$*

$$Q^n(f^n) \rightharpoonup Q(f) \ \ in \ \ L^1]0,m[\ \ as \ \ n \to \infty.$$

Proof. Let χ denotes the characteristic function. Choose $m > 0$ and let $\phi \in L^\infty]0, \infty[$. We show that $Q_i^n(f^n) \rightharpoonup Q_i(f)$ in $L^1]0, m[$ as $n \to \infty$ for $i = 1, 2, 3, 4$.

Case $i = 1$

For $f \in X^+$ and $x \in]0, m]$ define the operator h_1 by

$$h_1(f)(x) = \frac{1}{2} \int_0^{m-x} \phi(x+y) K(x, y) f(y) dy.$$

Assume $\phi \neq 0$. It can be easily shown that

$$\begin{aligned}
\int_0^m \phi(x) Q_1^n(f^n)(x) dx &= \frac{1}{2} \int_0^m \phi(x) \int_0^x K(x-y, y) f^n(x-y) f^n(y) dy dx \\
&= \frac{1}{2} \int_0^m \int_y^m \phi(x) K(x-y, y) f^n(x-y) f^n(y) dx dy \\
&= \frac{1}{2} \int_0^m \int_0^{m-y} \phi(y+x) K(x, y) f^n(x) f^n(y) dx dy \\
&= \frac{1}{2} \int_0^m \int_0^{m-x} \phi(x+y) K(x, y) f^n(x) f^n(y) dy dx \\
&= \frac{1}{2} \int_0^m f^n(x) \int_0^{m-x} \phi(x+y) K(x, y) f^n(y) dy dx \\
&= \int_0^m f^n(x) h_1(f^n)(x) dx. \qquad (2.24)
\end{aligned}$$

Note that for a.e. $x \in]0, m]$ we have

$$\frac{1}{2} \chi_{]0, m-x]}(\cdot) \phi(x + \cdot) K(x, \cdot) \in L^\infty]0, \infty[.$$

Since $f^n \rightharpoonup f$ in $L^1]0, \infty[$, it thus follows that

$$h_1(f^n)(x) \to h_1(f)(x) \quad \text{as} \quad n \to \infty \quad \text{for a.e.} \quad x \in]0, m]. \qquad (2.25)$$

We have

$$\begin{aligned}
|h_1(f^n)(x))| &= \left|\frac{1}{2}\int_0^{m-x} \phi(x+y)K(x,y)f^n(y)dy\right| \\
&\leq \frac{1}{2}\int_0^{m-x} |\phi(x+y)|K(x,y)f^n(y)dy \\
&\leq \frac{1}{2}||\phi||_{L^\infty]0,m[}\int_0^{m-x} K(x,y)f^n(y)dy \\
&\leq \frac{1}{2}||\phi||_{L^\infty]0,m[}k_1^2\int_0^{m} (1+x)^\mu(1+y)^\mu f^n(y)dy \\
&\leq \frac{1}{2}||\phi||_{L^\infty]0,m[}k_1^2(1+m)^\mu\int_0^{m} (1+y)^\mu f^n(y)dy \\
&\leq \frac{1}{2}||\phi||_{L^\infty]0,m[}k_1^2(1+m)^\mu L \quad \text{for a.e.} \quad x\in]0,m]. \qquad (2.26)
\end{aligned}$$

This is similarly true for $h_1(f)(x)$. Thus $h_1(f^n)$ and $h_1(f)$ belong to $L^\infty]0,m[$.
It now follows by (2.25) and Egoroff's Theorem [3, Theorem 2.5.5] that

$$h_1(f^n) \to h_1(f) \quad \text{as} \quad n\to\infty \quad \text{almost uniformly on} \quad x\in]0,m]. \qquad (2.27)$$

In other words, for a given $\delta > 0$ there exists a set $A \subseteq]0,m]$ such that $\lambda(A) < \delta$ and

$$h_1(f^n) \to h_1(f) \quad \text{uniformly on} \quad]0,m]\setminus A.$$

Choose $\epsilon > 0$. By Lemma 2.2.1(iii) there is a $\delta > 0$ such that for all n

$$\int_E f^n(x)dx < \epsilon/||\phi||_{L^\infty]0,m[}k_1^2(1+m)^\mu L \qquad (2.28)$$

whenever $\lambda(E) < \delta$. By (2.27), there is a set $A \subseteq]0,m]$ such that $\lambda(A) < \delta$ and $h_1(f^n) \to h_1(f)$ uniformly on $]0,m]\setminus A$. Thus

$$h_1(f^n) \to h_1(f) \quad \text{in} \quad L^\infty(]0,m]\setminus A) \quad \text{as} \quad n\to\infty. \qquad (2.29)$$

We now have, using Hölders inequality

$$\begin{aligned}
&\left|\int_0^m f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx\right| \\
&\qquad \leq \left|\int_{]0,m]\setminus A} f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx\right| \\
&\qquad\quad + \left|\int_A f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx\right| \\
&\qquad \leq ||h_1(f^n) - h_1(f)||_{L^\infty(]0,m]\setminus A)} \cdot \int_{]0,m]\setminus A} f^n(x)dx \\
&\qquad\quad + ||h_1(f^n) - h_1(f)||_{L^\infty(A)}\int_A f^n(x)dx.
\end{aligned}$$

Now considering (2.26) and (2.28) we obtain

$$\begin{aligned}
&||h_1(f^n) - h_1(f)||_{L^\infty(A)} \int_A f^n(x)dx \\
&\qquad = \sup_{x\in A} |h_1(f^n)(x) - h_1(f)(x)| \int_A f^n(x)dx \\
&\qquad \le \sup_{x\in A}\{|h_1(f^n)(x)| + |h_1(f)(x)|\} \int_A f^n(x)dx \\
&\qquad \le ||\phi||_{L^\infty]0,m[} k_1^2(1+m)^\mu L \cdot \epsilon / \{||\phi||_{L^\infty]0,m[} k_1^2(1+m)^\mu L\} \\
&\qquad \le \epsilon.
\end{aligned}$$

This together with Lemma 2.2.1 (i) leads to

$$\begin{aligned}
&\left| \int_0^m f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx \right| \\
&\qquad \le ||h_1(f^n) - h_1(f)||_{L^\infty(]0,m]\setminus A)} L + \epsilon \to \epsilon \quad \text{as} \quad n \to \infty.
\end{aligned}$$

Since $\epsilon > 0$ is arbitrary and with (2.29) we see that

$$\left| \int_0^m f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx \right| \to 0 \quad \text{as} \quad n \to \infty. \tag{2.30}$$

Due to $h_1(f) \in L^\infty]0,m[$ and $f^n \rightharpoonup f$ in $L^1]0,\infty[$ as $n \to \infty$ the definition of weak convergence implies that

$$\left| \int_0^m \{f^n(x) - f(x)\}h_1(f)(x)dx \right| \to 0 \quad \text{as} \quad n \to \infty. \tag{2.31}$$

It now follows by (2.24), (2.30) and (2.31) that

$$\begin{aligned}
&\left| \int_0^m \phi(x)\{Q_1^n(f^n)(x) - Q_1(f)(x)\}dx \right| \\
&\qquad \le \left| \int_0^m f^n(x)h_1(f^n)(x)dx - \int_0^m f^n(x)h_1(f)(x)dx \right. \\
&\qquad \left. + \int_0^m f^n(x)h_1(f)(x)dx - \int_0^m f(x)h_1(f)(x)dx \right| \\
&\qquad = \left| \int_0^m f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx + \int_0^m \{f^n(x) - f(x)\}h_1(f)(x)dx \right| \\
&\qquad \le \left| \int_0^m f^n(x)\{h_1(f^n)(x) - h_1(f)(x)\}dx \right| + \left| \int_0^m \{f^n(x) - f(x)\}h_1(f)(x)dx \right| \\
&\qquad \to 0 \quad \text{as} \quad n \to \infty.
\end{aligned} \tag{2.32}$$

Thus by the arbitrariness of ϕ it follows that

$$Q_1^n(f^n) \rightharpoonup Q_1(f) \quad \text{in} \quad L^1]0,m[\quad \text{as} \quad n \to \infty. \tag{2.33}$$

Case $i = 2$

Choose $\epsilon > 0$ and an arbitrary $\phi \in L^\infty]0,\infty[$. By (H3) we have $0 \leq \mu < 1$ and we can therefore choose $r > 0$ large enough such that

$$2k_1^2 L^2 ||\phi||_{L^\infty]0,m[}(1+r)^{\mu-1} < \epsilon. \tag{2.34}$$

For $f \in X^+$ and $x \in]0,m]$ we define the operator h_2 by

$$h_2(f)(x) = \int_0^r \phi(x)K(x,y)f(y)dy. \tag{2.35}$$

For a.e. $x \in]0,m]$ the function ϕ_x is defined by

$$\phi_x = \chi_{[0,r]}(\cdot)\phi(x)K(x,\cdot) \in L^\infty]0,\infty[.$$

By a similar argument to that used in (2.25)-(2.30) it can also be shown that (2.30) and (2.31) hold for the above defined h_2. By Lemma 2.2.1 (i), (2.34), and (H3)

$$\begin{aligned}
&\left| \int_0^m \int_r^\infty \phi(x)K(x,y)\{f^n(x)f^n(y) - f(x)f(y)\}dydx \right| \\
&\qquad \leq k_1^2 \int_0^m \int_r^\infty |\phi(x)|(1+x)^\mu(1+y)^\mu\{f^n(x)f^n(y) + f(x)f(y)\}dydx \\
&\qquad \leq k_1^2 \|\phi\|_{L^\infty]0,m[} L \left\{ \int_r^\infty \{(1+y)/(1+y)^{1-\mu}\}\{f^n(y) + f(y)\}dy \right\} \\
&\qquad \leq k_1^2 \|\phi\|_{L^\infty]0,m[} 2L^2(1+r)^{\mu-1} \\
&\qquad < \epsilon.
\end{aligned} \tag{2.36}$$

Also, for $n > m$,

$$\begin{aligned}
&\left| \int_0^m \int_{n-x}^\infty \phi(x)K(x,y)f^n(x)f^n(y)dydx \right| \\
&\qquad \leq k_1^2 \int_0^m \int_{n-x}^\infty |\phi(x)|(1+x)^\mu(1+y)^\mu f^n(x)f^n(y)dydx \\
&\qquad \leq k_1^2 \|\phi\|_{L^\infty]0,m[} \int_0^m (1+x)^\mu f^n(x)dx \int_{n-m}^\infty (1+y)^\mu f^n(y)dy \\
&\qquad \leq k_1^2 \|\phi\|_{L^\infty]0,m[} L \int_{n-m}^\infty \{(1+y)/(1+y)^{1-\mu}\} f^n(y)dy \\
&\qquad \leq k_1^2 \|\phi\|_{L^\infty]0,m[} L^2(1+n-m)^{\mu-1}.
\end{aligned}$$

It implies

$$\left| \int_0^m \int_{n-x}^\infty \phi(x)K(x,y)f^n(x)f^n(y)dydx \right| \to 0 \quad as \quad n \to \infty. \tag{2.37}$$

By using (2.35), (H3) and the analogues of (2.30) and (2.31),

$$\begin{aligned}
&\left|\int_0^m \int_0^r \phi(x)K(x,y)\{f^n(x)f^n(y) - f(x)f(y)\}dydx\right| \\
&\quad = \left|\int_0^m [f^n(x)h_2(f^n)(x) - f(x)h_2(f)(x)]dx\right| \\
&\quad = \left|\int_0^m [f^n(x)\{h_2(f^n)(x) - h_2(f)(x)\} + \{f^n(x) - f(x)\}h_2(f)(x)]dx\right| \\
&\quad \le \left|\int_0^m f^n(x)\{h_2(f^n)(x) - h_2(f)(x)\}dx\right| + \left|\int_0^m \{f^n(x) - f(x)\}h_2(f)(x)dx\right| \\
&\quad \to 0 \ \ as \ \ n \to \infty. \qquad (2.38)
\end{aligned}$$

It follows by (2.36), (2.37) and (2.38), for $n > m$

$$\begin{aligned}
&\left|\int_0^m \phi(x)\{Q_2^n(f^n)(x) - Q_2(f)(x)\}dx\right| \\
&\quad = \Bigg|\int_0^m \int_0^r \phi(x)K(x,y)\{f^n(x)f^n(y) - f(x)f(y)\}dydx \\
&\quad\quad + \int_0^m \int_r^\infty \phi(x)K(x,y)\{f^n(x)f^n(y) - f(x)f(y)\}dydx \\
&\quad\quad - \int_0^m \int_{n-x}^\infty \phi(x)K(x,y)f^n(x)f^n(y)dydx\Bigg| \\
&\quad \to \epsilon \ \ as \ \ n \to \infty.
\end{aligned}$$

Thus by the arbitrariness of ϕ and ϵ we have

$$Q_2^n(f^n) \rightharpoonup Q_2(f) \ \ in \ \ L^1]0,m[\ \ \text{as} \ \ n \to \infty. \qquad (2.39)$$

Case $i = 3$

For a.e. $x \in]0,m]$, by using (H4) we find that

$$|\phi(x)S(x)| \le k_2||\phi||_{L^\infty]0,m[}(1+m)^\gamma.$$

Then

$$\chi_{]0,m[}\phi S \in L^\infty]0,\infty[. \qquad (2.40)$$

Thus by (2.40) and since $f^n \rightharpoonup f$ in $L^1]0,\infty[$ as $n \to \infty$,

$$\begin{aligned}
&\left|\int_0^m \phi(x)\{Q_3^n(f^n)(x) - Q_3(f)(x)\}dx\right| \\
&\quad = \left|\int_0^m \phi(x)S(x)\{f^n(x) - f(x)\}dx\right| \to 0 \ \ \text{as} \ \ n \to \infty.
\end{aligned}$$

Since ϕ is arbitrary

$$Q_3^n(f^n) \rightharpoonup Q_3(f) \ \ in \ \ L^1]0,m[\ \text{ as } \ n \to \infty. \tag{2.41}$$

Case $i = 4$

Choose $\epsilon > 0$. By (H4) we have $0 \leq \gamma < 1$ and we can therefore choose $r > m$ such that for N given by (2.4)

$$2k_2 N \|\phi\|_{L^\infty]0,m[} L(1+r)^{\gamma-1} < \epsilon. \tag{2.42}$$

Then by Fubini's theorem, (H4) and (2.42)

$$\begin{aligned}
&\left| \int_0^m \int_r^\infty \phi(x) b(x,y) S(y)\{f^n(y) - f(y)\} dy dx \right| \\
&\qquad = \left| \int_r^\infty \int_0^m \phi(x) b(x,y) S(y) \{f^n(y) - f(y)\} dx dy \right| \\
&\qquad \leq k_2 N \|\phi\|_{L^\infty]0,m[} \int_r^\infty (1+y)^\gamma \{f^n(y) + f(y)\} dy \\
&\qquad \leq 2k_2 N \|\phi\|_{L^\infty]0,m[} L(1+r)^{\gamma-1} < \epsilon.
\end{aligned} \tag{2.43}$$

Also, for a.e. $x \in]0,m]$ the function

$$\chi_{]x,r]}(\cdot)\phi(x) S(\cdot) b(x,\cdot) = \chi_{]x,r]}(\cdot)\phi(x)\Gamma(\cdot,x) \in L^\infty]0,\infty[.$$

Thus, since $f^n \rightharpoonup f$ in $L^1]0,\infty[$, for a.e. $x \in]0,m]$

$$\phi(x) \int_x^r S(y) b(x,y)\{f^n(y) - f(y)\} dy \to 0 \ \text{ as } \ n \to \infty. \tag{2.44}$$

For a.e. $x \in]0,m]$ we take $k_3 = \sup_{\substack{x<y\leq r \\ 0<x\leq m}} \Gamma(y,x)$ and by using Lemma 2.2.1 (i)

$$\begin{aligned}
&|\phi(x)| \left| \int_x^r S(y) b(x,y) \{f^n(y) - f(y)\} dy \right| \\
&\qquad = |\phi(x)| \left| \int_x^r \Gamma(y,x) \{f^n(y) - f(y)\} dy \right| \\
&\qquad \leq k_3 \|\phi\|_{L^\infty]0,m[} \int_x^r \{|f^n(y)| + |f(y)|\} dy \\
&\qquad \leq k_3 \|\phi\|_{L^\infty]0,m[} \cdot 2L.
\end{aligned} \tag{2.45}$$

As a function of x this belongs to $L^1]0,m]$. Hence by (2.44), (2.45) and the dominated convergence theorem

$$\left| \int_0^m \int_x^r \phi(x) S(y) b(x,y) \{f^n(y) - f(y)\} dy dx \right| \to 0 \ \text{ as } \ n \to \infty.$$

Thus, by using Lemma 2.2.1 (i), (2.4), and (2.42) in the third integral on right-hand side, we obtain for $n \geq m$

$$\left| \int_0^m \phi(x)\{Q_4^n(f^n)(x) - Q_4(f)(x)\}dx \right|$$

$$= \left| \int_0^m \int_x^r \phi(x)S(y)b(x,y)\{f^n(y) - f(y)\}dydx \right.$$

$$+ \int_0^m \int_r^\infty \phi(x)b(x,y)S(y)\{f^n(y) - f(y)\}dydx$$

$$\left. - \int_0^m \int_n^\infty \phi(x)S(y)b(x,y)f^n(y)dydx \right|$$

$$\leq \left| \int_0^m \int_x^r \phi(x)S(y)b(x,y)\{f^n(y) - f(y)\}dydx \right| + \epsilon$$

$$+ k_2 N \|\phi\|_{L^\infty]0,m[} L(1+n)^{\gamma-1} \to \epsilon \quad \text{as} \quad n \to \infty.$$

By the arbitrariness of ϕ and ϵ, we obtain from above inequality

$$Q_4^n(f^n) \rightharpoonup Q_4(f) \quad in \quad L^1]0,m[\quad \text{as} \quad n \to \infty. \tag{2.46}$$

Lemma 2.2.2 follows from (2.33), (2.39), (2.41) and (2.46).

□

2.2.4 The existence theorem

Now we are in a position to state and prove the main result.

Theorem 2.2.3. *Suppose that (H1), (H2), (H3) and (H4) hold and assume that $f_0 \in X^+$. Then (2.1) has a solution f on $]0,\infty[$.*

Proof. Choose $m > 0$, $T > 0$, and let $(f^n)_{n\in\mathbb{N}}$ be the subsequence of approximating solutions obtained above. We have from subsection 2.2.1, for $t \in [0,T]$

$$f^n(t) \rightharpoonup f(t) \quad in \quad L^1]0,m[\quad \text{as} \quad n \to \infty. \tag{2.47}$$

For any $l > 0$, since we know $f^n \rightharpoonup f$ in $L^1]0,\infty[$, we obtain

$$\int_0^l xf(x,t)dx = \lim_{n\to\infty} \int_0^l xf^n(x,t)dx \leq \|f_0\|_x < \infty \tag{2.48}$$

using (2.8), the non-negativity of each f^n and f, and then $l \to \infty$ implies that $f \in X^+$. Let $\phi \in L^\infty]0,m[$. From Lemma 2.2.2 we have for each $s \in [0,t]$

$$\int_0^m \phi(x)\{Q^n(f^n(s))(x) - Q(f(s))(x)\}dx \to 0 \ \ as \ \ n \to \infty. \tag{2.49}$$

Also, for $s \in [0,t]$, using Young's Theorem for convolutions and Lemma 2.2.1 (i)

$$\begin{aligned}
&\int_0^m |\phi(x)||Q^n(f^n(s))(x) - Q(f(s))(x)|dx \\
&\leq \|\phi\|_{L^\infty]0,m[}\Big\{\frac{1}{2}\int_0^m\int_0^x K(x-y,y)\{f^n(x-y,s)f^n(y,s) + f(x-y,s)f(y,s)\}dydx \\
&+ \int_0^m\int_0^{n-x} K(x,y)f^n(x,s)f^n(y,s)dydx + \int_0^m\int_0^\infty K(x,y)f(x,s)f(y,s)dydx \\
&+ \int_0^m S(x)\{f^n(x,s) + f(x,s)\}dx \\
&+ \int_0^m\int_x^n S(y)b(x,y)f^n(y,s)dydx + \int_0^m\int_x^\infty S(y)b(x,y)f(y,s)dydx\Big\} \\
&\leq \|\phi\|_{L^\infty]0,m[}\{3k_1^2L^2 + 2k_2(N+1)L\}.
\end{aligned} \tag{2.50}$$

Since the left-hand side of (2.50) is in $L^1]0,t[$ we have by (2.49), (2.50) and the dominated convergence theorem

$$\left|\int_0^t\int_0^m \phi(x)\{Q^n(f^n(s))(x) - Q(f(s))(x)\}dxds\right| \to 0 \ \text{ as } \ n \to \infty. \tag{2.51}$$

Since ϕ is arbitrary, and the equation (2.51) holds for all $\phi \in L^\infty]0,m[$, by the application of Fubini's Theorem we obtain

$$\int_0^t Q^n(f^n(s))ds \rightharpoonup \int_0^t Q(f(s))ds \ \text{ in } \ L^1]0,m[\ \text{ as } \ n \to \infty. \tag{2.52}$$

From the definition of Q^n and equation (2.6) we have for $t \in [0,T]$

$$f^n(x,t) = \int_0^t Q^n(f^n(s))(x)ds + f^n(x,0),$$

and thus it follows from (2.52)and (2.47) that

$$\int_0^m \phi(x)f(x,t)dx = \int_0^t\int_0^m \phi(x)Q(f(s))(x)dxds + \int_0^m \phi(x)f(x,0)dx, \tag{2.53}$$

for any $\phi \in L^\infty]0,m]$. Therefore it holds for all $\phi \in C_0^\infty(]0,m])$. This implies for almost any x in $]0,m]$ we have

$$f(x,t) = \int_0^t Q(f(s))(x)ds + f(x,0).$$

It now follows from the arbitrariness of T and m that f is a solution to (2.1) on $[0,\infty[$. This completes the proof of Theorem 2.2.3. □

Chapter 3

Uniqueness of solutions

In this chapter we take into account two different issues concerning uniqueness of solutions. First, the existence of at least one mass conserving solution for continuous coagulation and binary fragmentation equation has been established by Escobedo et al. [27] for a large class of coagulation kernels under strong binary fragmentation. In continuation of this, we investigate the uniqueness of mass conserving solutions with some additional restrictions on the fragmentation kernels. This work is motivated by Stewart [90] and Da Costa [14]. Secondly, to complement the existence of solutions for the coagulation and multiple fragmentation equation in Chapter 2, the uniqueness of solutions is again demonstrated under more stringent assumptions on the coagulation and fragmentation kernels.

The plan of this chapter is as follows. Section 3.1 recalls the coagulation and binary fragmentation equation from Chapter 1 and introduces some definitions, notations, a useful lemma as well as the statement of the existence theorem given by Escobedo et al. [27] for mass conserving solutions. Then, by proving the integrability of higher moments, we show the uniqueness of mass conserving solutions for coagulation equation with binary fragmentation in Section 3.2. Finally, Section 3.3 contains the uniquenss result for coagulation equation with multiple fragmentation. Before proceeding to the Section 3.3, it is recommended that readers review Chapter 2.

3.1 Introduction

The nonlinear continuous coagulation and fragmentation equation is given by

$$\frac{\partial f(x,t)}{\partial t} = \frac{1}{2}\int_0^x J(x-y,y,f(t))dy - \int_0^\infty J(x,y,f(t))dy \tag{3.1}$$

with initial data

$$f(x,0) = f_0(x) \geq 0. \tag{3.2}$$

The integral J is defined as

$$J(x, y, f(t)) = K(x, y)f(x, t)f(y, t) - F(x, y)f(x + y, t) \tag{3.3}$$

Let X be the following Banach space with norm $\|\cdot\|$

$$X = \{f \in L^1]0, \infty[: \|f\| < \infty\} \text{ where } \|f\| = \int_0^\infty (1 + x)|f(x)|dx$$

and set

$$X^+ = \{f \in X : f \geq 0 \ \ a.e.\}.$$

The rth moment of the number density distribution if it exists is defined by

$$M_r(t) = M_r(f(t)) := \int_0^\infty x^r f(x, t)dx, \quad r \in \mathbb{R}_{\geq 0}.$$

The first two moments represent some important properties of the distribution. The zeroth ($r = 0$) and first ($r = 1$) moments are proportional to the total number and the total mass of particles, respectively.

Definition 3.1.1. *Let $0 < T \leq \infty$. A solution f of (3.1) is a function $f : [0, T[\to X^+$ such that for a.e. $x \in [0, \infty[$ the following hold*

(i) $f(x, t) \geq 0$ for all $t \in [0, T[$,

(ii) $f(x, .)$ is continuous on $[0, T[$,

(iii) for all $t \in [0, T[$

$$\int_0^t \int_0^\infty K(x, y)f(y, s)dyds < \infty \quad \text{and} \quad \int_0^t \int_0^\infty F(x, y)f(x + y, s)dyds < \infty,$$

(iv) for all $t \in [0, T[$

$$f(x, t) = f(x, 0) + \int_0^t \left\{ \frac{1}{2} \int_0^x J(x - y, y, f(s))dy - \int_0^\infty J(x, y, f(s))dy \right\} ds.$$

Lemma 3.1.2. *Let $r : \mathbb{R}^2_{\geq 0} \times]0, \infty[\mapsto \mathbb{R}_{\geq 0}$ be a real-valued function and*

$$\int_0^t \int_0^\infty \int_0^\infty r(x, y, s)dydxds < \infty \quad \text{for all} \quad t \in]0, T[.$$

Then

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty r(x, y, s)dydxds = 0.$$

Proof. We know that

$$\int_0^t \int_0^n \int_{n-x}^{\infty} r(x,y,s)dydxds = \int_0^t \int_0^{\infty} \int_0^{\infty} r(x,y,s)dydxds - \Big(\int_0^t \int_0^n \int_0^{n-x} r(x,y,s)dydxds + \int_0^t \int_n^{\infty} \int_0^{\infty} r(x,y,s)dydxds \Big).$$

This gives the inequality

$$0 \le \int_0^t \int_0^n \int_{n-x}^{\infty} r(x,y,s)dydxds \le \int_0^t \int_0^{\infty} \int_0^{\infty} r(x,y,s)dydxds - \int_0^t \int_0^n \int_0^{n-x} r(x,y,s)dydxds.$$

Passing the limit $n \to \infty$, by dominated convergence theorem we obtain

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^{\infty} r(x,y,s)dydxds = 0.$$

□

Remark 3.1.3. *A similar result as in Lemma 3.1.2 has been used by Dubovskii [21].*

Let $g : \mathbb{R} \to \mathbb{R}$ be any continuous function. For convenience we define the following integrals T_i, $i = 1$ to 4, for $a, b \in \mathbb{R}_{\geq 0}$ and $s \in [0, T[$:

$$T_1(a,b,s) = \frac{1}{2} \int_a^{b-a} \int_a^{b-x} [g(x+y) - g(x) - g(y)] J(x,y,f(s))dydx,$$

$$T_2(a,b,s) = \frac{1}{2} \int_0^a \int_{a-x}^a g(x+y) J(x,y,f(s))dydx,$$

$$T_3(a,b,s) = \int_0^a \int_a^{b-x} [g(x+y) - g(y)] J(x,y,f(s))dydx,$$

$$T_4(a,b,s) = -\int_a^b \int_{b-x}^{\infty} g(x) J(x,y,f(s))dydx.$$

From Lemma 2.1 in Stewart [91], which is also true for the coagulation-fragmentation equation, we have

$$\int_a^b g(x)f(x,t)dx - \int_a^b g(x)f(x,0)dx = \int_0^t \sum_{i=1}^4 T_i(a,b,s)ds. \tag{3.4}$$

Theorem 3.1.4. *Assume that the kernels satisfy the following hypotheses for existence:*
(H1): $K(x,y) \leq k[(1+x)^{\alpha}(1+y)^{\beta} + (1+x)^{\beta}(1+y)^{\alpha}]$ *for all* $x, y \in]0,\infty[$ *for some* $0 \leq \alpha \leq \beta \leq 1$ *and positive constant* k.
(H2): (i) For each $R \in \mathbb{R}_{>0}$ *there is a constant* $F_R > 0$ *such that*

$$F(x,y) \leq F_R \quad for \quad (x,y) \in]0,R[^2.$$

(ii) There are constants $R_0 > 0$, $S_0 \geq R_0$ *and* C_0 *such that*

$$\int_0^{R_0} F(y, x-y)dy \leq C_0 \int_0^{R_0} yF(y,x-y)dy \quad for\ any \quad x \geq S_0.$$

(iii) For $1 < \alpha + \beta \leq 2$, α, β *as in (H1), there are constants* $B_0 > 0$ *and* $\gamma > \alpha + \beta - 2$ *such that*

$$F(x-y,y) \geq B(x) := B_0(1+x)^{\gamma} \quad for\ any \quad x \geq 1 \quad and \quad y \in]0,x[. \tag{3.5}$$

Then for any initial data $f_0 \in X^+$, *there exists at least one mass conserving solution to the initial value problem (3.1-3.3).*

Proof. The proof can be found in Section 3 of Escobedo et al. [27]. □

The condition (H2)(iii) is called **strong fragmentation condition**. Thereby the theorem requires both $0 \leq \alpha \leq \beta \leq 1$ and $\alpha + \beta > 1$ to hold.

3.2 Uniqueness for coagulation and binary fragmentation equation

In order to prove the uniqueness, we consider the hypotheses (H1) with the following restriction on (H2) i.e. (H2')

(H2'): (i) there exists a $C > 0$ such that

$$\int_0^x F(x-y,y)dy \leq C(1+x) \quad \text{for all} \quad x > 0.$$

(ii) There are constants B_0 and $\gamma > -1$ such that (3.5) holds.

To prove the uniqueness, we require the integrability of higher moments M_λ, the moment of order λ of f where $\lambda \in]1,2]$ i.e.

$$\int_0^t M_\lambda(f(s))ds < \infty \quad \text{for all} \quad t \in [0,T[$$

3.2.1 Integrability of higher moments

First we introduce a new class of kernels both for coagulation and fragmentation.

Hypotheses 3.2.1. *(HM1)* $K(x,y) \leq k_1(1+x)^{\beta}(1+y)^{\beta}$ *for some* $0 \leq \beta \leq 1$.

(HM2) There are constants $B_0 > 0$ *and* $\gamma > -1$ *such that*

$$F(x-y,y) \geq B(x) := B_0(1+x)^{\gamma} \quad \text{for any} \quad x \geq 1 \quad \text{and} \quad y \in]0,x[.$$

Note that the class of kernels satisfying (HM1) is larger than that satisfying (H1). This is typical for the combined coagulation-fragmentation problem. There is always a trade off between the hypotheses.

Theorem 3.2.2. *Assume (HM1) and (HM2) hold. Let* $f \in X^+$ *be any solution of equation (3.1) on* $[0,T[$, $T > 0$. *Then, for every* $t \in [0,T[$ *and for every* $\epsilon > 0$,

$$\int_0^t M_{2+\gamma-\epsilon}(f(s))ds < \infty.$$

The proof of Theorem 3.2.2 consists of a repeated application of the following Lemma:

Lemma 3.2.3. *Assume (HM1) and (HM2) hold. Let* $f \in X^+$ *be any solution of equation (3.1) on* $[0,T[$, $T > 0$, *and assume*

$$\int_0^t M_{\sigma}(f(s))ds < \infty \quad \text{for all} \quad t \in [0,T[\quad \text{and some} \quad \sigma \geq 1 \quad \text{with} \quad \sigma > \beta.$$

Then, with $1+\gamma > \beta$, *for all* $t \in [0,T[$,

$$\int_0^t M_{\sigma+\gamma-\beta+1}(f(s))ds < \infty \quad \text{if} \quad \sigma - \beta < 1.$$

In case $\sigma - \beta \geq 1$ *we obtain*

$$\int_0^t M_{2+\gamma-\epsilon}(f(s))ds < \infty \quad \text{for any} \quad \epsilon > 0.$$

Proof. We know from equation (3.4) that for any continuous function $g : \mathbb{R} \to \mathbb{R}$,

$$\int_a^b g(x)f(x,t)dx - \int_a^b g(x)f(x,0)dx = \int_0^t \sum_{i=1}^{4} T_i(a,b,s)ds.$$

Let us take some $\lambda \in [0,1[$ and substitute $g(x) = x^\lambda$, $a = 0$ and $b = n$ to get

$$\begin{aligned}
&\int_0^n x^\lambda [f(x,t) - f_0(x)]dx \\
&\quad + \int_0^t \left[\frac{1}{2} \int_0^n \int_0^{n-x} \{x^\lambda + y^\lambda - (x+y)^\lambda\} K(x,y) f(x,s) f(y,s) dy dx \right. \\
&\quad \left. + \int_0^n \int_{n-x}^\infty x^\lambda K(x,y) f(x,s) f(y,s) dy dx \right] ds \\
&= \int_0^t \left[\frac{1}{2} \int_0^n \int_0^{n-x} \{x^\lambda + y^\lambda - (x+y)^\lambda\} F(x,y) f(x+y,s) dy dx \right. \\
&\quad \left. + \int_0^n \int_{n-x}^\infty x^\lambda F(x,y) f(x+y,s) dy dx \right] ds. \qquad (3.6)
\end{aligned}$$

Since $\lambda < 1$ and $f \in X^+$, the first term on the left hand side is bounded independently of n and is convergent as $n \to \infty$. For the last term on the left hand side, we have

$$\begin{aligned}
&\int_0^t \int_0^n \int_0^n x^\lambda K(x,y) f(x,s) f(y,s) dy dx ds \\
&\quad \le k_1 \int_0^t \int_0^n \int_0^n x^\lambda (1+x)^\beta (1+y)^\beta f(x,s) f(y,s) dy dx ds \\
&\quad = k_1 \int_0^t \int_0^n \int_0^1 x^\lambda (1+x)^\beta (1+y)^\beta f(x,s) f(y,s) dy dx ds \\
&\qquad + k_1 \int_0^t \int_0^n \int_1^n x^\lambda (1+x)^\beta (1+y)^\beta f(x,s) f(y,s) dy dx ds \\
&\quad = 2^\beta k_1 \int_0^t \int_0^n \int_0^1 x^\lambda (1+y) f(x,s) f(y,s) dy dx ds \\
&\qquad + 2^\beta k_1 \int_0^t \int_0^n \int_1^n x^{\lambda+\beta} (1+y) f(x,s) f(y,s) dy dx ds.
\end{aligned}$$

Now in case $\lambda + \beta \le \sigma$ we obtain

$$\begin{aligned}
&\int_0^t \int_0^n \int_0^n x^\lambda K(x,y) f(x,s) f(y,s) dy dx ds \\
&\qquad \le 2^\beta k_1 \max_{s \in [0,t]} \|f(s)\| \int_0^t [M_\lambda(f(s)) + M_\sigma(f(s))] ds < \infty. \qquad (3.7)
\end{aligned}$$

Now we consider the second term on the left hand side of equation (3.6) as follows

$$\begin{aligned}
\frac{1}{2}\int_0^t\int_0^n\int_0^n &\{x^\lambda + y^\lambda - (x+y)^\lambda\}K(x,y)f(x,s)f(y,s)dydxds \\
&\leq \frac{k_1}{2}\int_0^t\int_0^n\int_0^n (x^\lambda + y^\lambda)(1+x)^\beta(1+y)^\beta f(x,s)f(y,s)dydxds \\
&\leq k_1\int_0^t\int_0^n\int_0^n x^\lambda(1+x)^\beta(1+y)^\beta f(x,s)f(y,s)dydxds \\
&\leq 2^\beta k_1 \max_{s\in[0,t]}\|f(s)\|\int_0^t [M_\lambda(f(s)) + M_\sigma(f(s))]ds < \infty.
\end{aligned}$$

Hence the left hand side of (3.6) converges as $n \to \infty$ and so does the right hand side. Since all the terms in it are non-negative, this implies that

$$\int_0^t\int_0^\infty\int_0^\infty \{x^\lambda + y^\lambda - (x+y)^\lambda\}F(x,y)f(x+y,s)dydxds < \infty. \tag{3.8}$$

Let us take the integral

$$\int_0^\infty\int_0^\infty \{x^\lambda + y^\lambda - (x+y)^\lambda\}F(x,y)f(x+y,s)dydx.$$

By changing the order of integration and making a change of variable $x + y = x'$, $y = y'$ we obtain

$$\int_0^\infty\int_{y'}^\infty \{(x'-y')^\lambda + y'^\lambda - x'^\lambda\}F(x'-y',y')f(x',s)dx'dy'.$$

Again changing the order of integration and drop the primes to get

$$\begin{aligned}
\int_0^\infty\int_0^x &\{(x-y)^\lambda + y^\lambda - x^\lambda\}F(x-y,y)f(x,s)dydx \\
&= \int_0^\infty B_x f(x,s)dx \\
&\quad \text{where } \ B_x = \int_0^x \{(x-y)^\lambda + y^\lambda - x^\lambda\}F(x-y,y)dy.
\end{aligned}$$

Note that the integral B_x is non-negative due to $\lambda \in [0,1[$ and $y \in [0,x]$. In Proposition A.0.6 we take $y' = \frac{x}{2}$. Then there exists a constant $k_\lambda > 0$ for each $\lambda \in [0,1[$ such that

$$y^\lambda + (x-y)^\lambda - x^\lambda \geq k_\lambda y^\lambda$$

and

$$\begin{aligned}
B_x &\geq \int_0^{x/2} \{(x-y)^\lambda + y^\lambda - x^\lambda\}F(x-y,y)dy \\
&\geq k_\lambda \int_0^{x/2} y^\lambda F(x-y,y)dy.
\end{aligned} \tag{3.9}$$

Using (HM2) in (3.9) we get

$$\begin{aligned} B_x &\geq B_0 \frac{k_\lambda}{\lambda+1}(1+x)^\gamma (\frac{x}{2})^{\lambda+1} \\ &= B_0 k'_\lambda \frac{(1+x)^{\gamma+1}}{(\frac{1}{x}+1)} x^\lambda \\ &\geq \frac{B_0}{2} k'_\lambda x^{\gamma+\lambda+1} \quad \text{for any} \quad x \geq 1. \end{aligned} \tag{3.10}$$

Substituting (3.10) for B_x and then into (3.8) we obtain

$$\begin{aligned} &\frac{B_0}{2} k'_\lambda \int_0^t \int_0^\infty x^{\gamma+\lambda+1} f(x,s) dx ds \\ &\qquad \leq \int_0^t \int_0^\infty \int_0^\infty \{x^\lambda + y^\lambda - (x+y)^\lambda\} F(x,y) f(x+y,s) dy dx ds < \infty. \end{aligned}$$

There are two cases. For $\sigma - \beta < 1$ we may take the maximal $\lambda = \sigma - \beta$ to give

$$\int_0^t M_{\sigma+\gamma-\beta+1}(f(s)) ds < \infty.$$

Otherwise the condition $\lambda < 1$ is more restrictive, i.e. we may take $\lambda = 1 - \epsilon$ for any $\epsilon > 0$. This gives

$$\int_0^t M_{\gamma+2-\epsilon}(f(s)) ds < \infty.$$

□

Proof of Theorem 3.2.2. Let p be the smallest positive integer satisfying

$$p(\mu - \beta) > \beta \quad \text{where} \quad \mu := 1 + \gamma > \beta.$$

(a) If $p > 1$. Then $p - 1$ is a positive integer and

$$0 < (p-1)(\mu - \beta) < \beta.$$

Now we define $\sigma_i := 1 + (i-1)(\mu - \beta)$ to have

$$1 = \sigma_1 < \sigma_2 < \ldots < \sigma_{p-1} < \sigma_p < 1 + \beta.$$

Applying Lemma 3.2.3 p times, starting with $\sigma = \sigma_1 = 1$, gives

$$\int_0^t M_{\sigma_{p+1}}(f(s)) ds < \infty,$$

and one more application of Lemma 3.2.3 with $\sigma = \sigma_{p+1} = 1 + p(\mu - \beta) > 1$ proves the result.

(b) If $p = 1$. Then we start with $\sigma = 1$ and apply Lemma 3.2.3 two times to obtain the result.

Theorem 3.2.4. *Let f be a mass conserving solution of equation (3.1) subject to (3.2), (3.3) with initial data $f_0 \in X^+$. If the hypotheses (H1) and (H2') hold, then the solution is unique.*

Proof. For $q \in \mathbb{R}$, define $\text{sgn}(q)$ equal to 1, 0, -1 whenever $q > 0$, $q = 0$ or $q < 0$ respectively. Let f_1 and f_2 be two solutions to (3.1-3.3) on $[0, T[$, where $T > 0$, with $f_1(0) = f_2(0)$, and set $Y = f_1 - f_2$. For $n = 1, 2, 3, \ldots$, we define

$$u^n(t) := \int_0^n (1+x)|Y(x,t)|dx. \tag{3.11}$$

Multiplying $|Y|$ by $(1+x)$ and applying Fubini's theorem to Definition 3.1.1 (iv) above, we obtain for each n and $0 < t < T$,

$$u^n(t) = \int_0^t \int_0^n (1+x)\text{sgn}(Y(x,s)) \Bigg[\frac{1}{2}\int_0^x \Big(J(x-y,y,f_1(s)) - J(x-y,y,f_2(s))\Big)dy \\ - \int_0^\infty \Big(J(x,y,f_1(s)) - J(x,y,f_2(s))\Big)dy\Bigg]dxds. \tag{3.12}$$

Using the substitution $x' = x - y$, $y' = y$ in the first integral on the right hand side of (3.12), we find that

$$u^n(t) = \int_0^t \int_0^n \int_0^{n-x} \Big[\frac{1}{2}(1+x+y)\text{sgn}(Y(x+y,s)) - (1+x)\text{sgn}(Y(x,s))\Big] \\ \times \Big[J(x,y,f_1(s)) - J(x,y,f_2(s))\Big]dydxds \\ - \int_0^t \int_0^n \int_{n-x}^\infty (1+x)\text{sgn}(Y(x,s))\Big[J(x,y,f_1(s)) - J(x,y,f_1(s))\Big]dydxds. \tag{3.13}$$

By interchanging the order of integration (and interchanging the roles of x and y), the symmetry of J yields the identity

$$\int_0^n \int_0^{n-x} (1+x)\text{sgn}(Y(x,s))J(x,y,f_1(s))dydx \\ = \int_0^n \int_0^{n-x} (1+y)\text{sgn}(y(x,s))J(x,y,f_1(s))dydx. \tag{3.14}$$

The equation (3.14) analogously holds for solution f_2. For $x, y \geq 0$ and $t \in [0, T[$, define c by

$$c(x,y,t) = (1+x+y)\text{sgn}(Y(x+y,t)) - (1+x)\text{sgn}(Y(x,t)) - (1+y)\text{sgn}(Y(y,t)).$$

Using (3.14) we can show that (3.13) can be rewritten as

$$\begin{aligned} u^n(t) =& \frac{1}{2}\int_0^t \int_0^n \int_0^{n-x} c(x,y,s)K(x,y)f_1(x,s)Y(y,s)dydxds \\ &+ \frac{1}{2}\int_0^t \int_0^n \int_0^{n-x} c(x,y,s)K(x,y)f_2(y,s)Y(x,s)dydxds \\ &- \frac{1}{2}\int_0^t \int_0^n \int_0^{n-x} c(x,y,s)F(x,y)Y(x+y,s)dydxds \\ &- \int_0^t \int_0^n \int_{n-x}^{\infty} (1+x)\text{sgn}(Y(x,s))\Big[J(x,y,f_1(s)) - J(x,y,f_2(s))\Big]dydxds. \\ =:& \int_0^t \sum_{i=1}^{4} S_i^n(s)ds. \end{aligned}$$

Here S_i^n, for $i = 1,2,3,4$ are the corresponding integrands in the preceding lines.

We now consider each S_i^n individually. Note that for all $q, q_1, q_2 \in \mathbb{R}$, we have

$$\text{sgn}(q_1)\text{sgn}(q_2) = \text{sgn}(q_1q_2) \quad \text{and} \quad |q| = q\text{sgn}(q).$$

We find that

$$c(x,y,s)Y(y,s) \leq \Big[(1+x+y) + (1+x) - (1+y)\Big]|Y(y,s)| = 2(1+x)|Y(y,s)|. \quad (3.15)$$

Now, we consider

$$\begin{aligned} &\int_0^t S_1^n(s)ds \\ &\quad = \frac{1}{2}\int_0^t \int_0^n \int_0^{n-x} c(x,y,s)K(x,y)f_1(x,s)Y(y,s)dydxds \\ &\quad \leq k\int_0^t \int_0^n \int_0^{n-x} (1+x)[(1+x)^{\alpha}(1+y)^{\beta} + (1+x)^{\beta}(1+y)^{\alpha}]f_1(x,s)|Y(y,s)|dydxds \\ &\quad \leq 2k\int_0^t \int_0^n \int_0^{n-x} (1+x)^{1+\beta}(1+y)^{\beta}f_1(x,s)|Y(y,s)|dydxds \\ &\quad \leq 2k\int_0^t \left[\int_0^1 (1+x)^{1+\beta}f_1(x,s)dx + \int_1^n x^{1+\beta}(\frac{1}{x}+1)^{1+\beta}f_1(x,s)dx\right]u^n(s)ds \\ &\quad = 2^{\beta+2}k\int_0^t [M_0(f_1(s)) + M_{1+\beta}(f_1(s))]u^n(s)ds \\ &\quad = \int_0^t \varphi_{f_1}(s)u^n(s)ds \end{aligned}$$

where

$$\varphi_{f_1}(s) := 2^{\beta+2}k[M_0(f_1(s)) + M_{1+\beta}(f_1(s))].$$

Similarly we define

$$\varphi_{f_2}(s) := 2^{\beta+2}k[M_0(f_2(s)) + M_{1+\beta}(f_2(s))]$$

to get

$$\int_0^t S_2^n(s)ds \leq \int_0^t \varphi_{f_2}(s)u^n(s)ds.$$

To solve S_3^n we use the following inequality

$$\begin{aligned}-c(x,y,s)Y(x+y,s) &\leq \Big[(1+x)+(1+y)-(1+x+y)\Big]|Y(x+y,s)| \\ &= |Y(x+y,s)|. \end{aligned} \tag{3.16}$$

By using (3.16), Fubini's theorem, hypothesis (H2') and the symmetry of F

$$\begin{aligned}\int_0^t S_3^n(s)ds &\leq \frac{1}{2}\int_0^t\int_0^n\int_0^{n-x} F(x,y)|Y(x+y,s)|dydxds \\ &= \frac{1}{2}\int_0^t\int_0^n\int_x^n F(x,y-x)|Y(y,s)|dydxds \\ &= \frac{1}{2}\int_0^t\int_0^n\int_0^y F(x,y-x)|Y(y,s)|dxdyds \\ &= \frac{1}{2}\int_0^t\int_0^n\int_0^x F(x-y,y)|Y(x,s)|dydxds \\ &\leq \frac{C}{2}\int_0^t\int_0^n (1+x)|Y(x,s)|dxds \\ &= \frac{C}{2}\int_0^t u^n(s)ds.\end{aligned}$$

Thus,

$$\int_0^t \Big[S_1^n(s)+S_2^n(s)+S_3^n(s)\Big]ds \leq \int_0^t \varphi(s)u^n(s)ds \tag{3.17}$$

where $\varphi(s) = \varphi_{f_1}(s) + \varphi_{f_2}(s) + \frac{C}{2}$ is integrable by Theorem 3.2.2. For the fourth term we have

$$\begin{aligned}&\left|\int_0^t S_4^n(s)ds\right| \\ &=\Bigg| -\int_0^t\int_0^n\int_{n-x}^{\infty}(1+x)\mathrm{sgn}(Y(x,s))\Big[K(x,y)f_1(x,s)f_1(y,s) - F(x,y)f_1(x+y,s) \\ &\quad - K(x,y)f_2(x,s)f_2(y,s) + F(x,y)f_2(x+y,s)\Big]dydxds\Bigg|.\end{aligned}$$

This gives the estimate

$$\begin{aligned}
&\left| \int_0^t S_4^n(s)ds \right| \\
&\quad \le \int_0^t \int_0^n \int_{n-x}^{\infty} \Big| (1+x)\mathrm{sgn}(Y(x,s))K(x,y)[f_1(x,s)f_1(y,s) - f_2(x,s)f_2(y,s)] \Big| dydxds \\
&\qquad + \int_0^t \int_0^n \int_{n-x}^{\infty} \Big| (1+x)\mathrm{sgn}(Y(x,s))F(x,y)Y(x+y,s) \Big| dydxds. \qquad (3.18)
\end{aligned}$$

For the first term on the right hand side in the above inequality we have

$$\begin{aligned}
&\int_0^t \int_0^\infty \int_0^\infty \Big| (1+x)\mathrm{sgn}(Y(x,s))K(x,y)[f_1(x,s)f_1(y,s) - f_2(x,s)f_2(y,s)] \Big| dydxds \\
&\quad \le k \int_0^t \int_0^\infty \int_0^\infty (1+x)[(1+x)^\alpha(1+y)^\beta + (1+x)^\beta(1+y)^\alpha] \\
&\qquad\qquad \times [f_1(x,s)f_1(y,s) + f_2(x,s)f_2(y,s)]dydxds \\
&\quad \le 2k \int_0^t \int_0^\infty \int_0^\infty (1+x)^{1+\beta}(1+y)^\beta[f_1(x,s)f_1(y,s) + f_2(x,s)f_2(y,s)]dydxds. \qquad (3.19)
\end{aligned}$$

Now we consider the first term on the right hand side of the above inequality (3.19).

$$\begin{aligned}
&2k \int_0^t \int_0^\infty \int_0^\infty (1+x)^{1+\beta}(1+y)^\beta f_1(x,s)f_1(y,s)dydxds \\
&= 2k \int_0^t \left[\int_0^1 (1+x)^{1+\beta} f_1(x,s)dx + \int_1^\infty x^{1+\beta}(1/x+1)^{1+\beta} f_1(x,s)dx \right] M_\beta(f_1(s))ds \\
&= 2^{\beta+2}k \int_0^t [M_0(f_1(s)) + M_{1+\beta}(f_1(s))]M_\beta(c(s))ds < \infty.
\end{aligned}$$

Similarly we can show the finiteness of the second term on the right hand side in (3.19). Note that we have used the integrability of higher moments of solutions f_1 and f_2. So, by using Lemma 3.1.2 we obtain

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^{\infty} \Big| (1+x)\mathrm{sgn}(Y(x,s))K(x,y)[f_1(x,s)f_1(y,s) - f_2(x,s)f_2(y,s)] \Big| dydxds = 0. \qquad (3.20)$$

For the second term on the right hand side in (3.18) we substitute $g(x) = x$, $a = 0$ and $b = n$ in equation (3.4), we obtain

$$\int_0^n x f_1(x,t)dx - \int_0^n x f_1(x,0)dx = - \int_0^t \int_0^n \int_{n-x}^{\infty} xJ(x,y,f_1(s))dydxds$$

Taking limit as $n \to \infty$,

$$\int_0^\infty x f_1(x,t) - \int_0^\infty x f_1(x,0)dx = -\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xJ(x,y,f_1(s))dydxds \tag{3.21}$$

Since f_1 and f_1 are mass conserving solutions we have from (3.21)

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xJ(x,y,f_1(s))dydxds = 0 \tag{3.22}$$

and similarly,

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xJ(x,y,f_2(s))dydxds = 0. \tag{3.23}$$

From equation (3.22), we obtain

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xK(x,y)f_1(x,s)f_1(y,s)dydxds$$
$$= \lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xF(x,y)f_1(x+y,s)dydxds.$$

By using same argument as used before we get

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xK(x,y)f_1(x,s)f_1(y,s)dydxds = 0.$$

This implies that

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xF(x,y)f_1(x+y,s)dydxds = 0. \tag{3.24}$$

Analogously, we have

$$\lim_{n\to\infty} \int_0^t \int_0^n \int_{n-x}^\infty xF(x,y)f_2(x+y,s)dydxds = 0. \tag{3.25}$$

Now we consider

$$\int_0^t \int_0^n \int_{n-x}^\infty \Big| x\mathrm{sgn}(Y(x,s))F(x,y)Y(x+y,s)\Big| dydxds$$
$$\le \int_0^t \int_0^n \int_{n-x}^\infty xF(x,y)|Y(x+y,s)|dydxds$$
$$\le \int_0^t \int_0^n \int_{n-x}^\infty xF(x,y)f_1(x+y,s)dydxds$$
$$+ \int_0^t \int_0^n \int_{n-x}^\infty xF(x,y)f_2(x+y,s)dydxds.$$

Using (3.24) and (3.25), we get

$$\lim_{n\to\infty}\int_0^t\int_0^n\int_{n-x}^\infty \Big| x\mathrm{sgn}(Y(x,s))F(x,y)Y(x+y,s)\Big| dydxds = 0. \tag{3.26}$$

Now we use the symmetry of F, Fubini's theorem and hypothesis (H2') to have for each $s \in [0,t]$,

$$\begin{aligned}
&\int_0^n\int_{n-x}^\infty \Big|\mathrm{sgn}(Y(x,s))F(x,y)Y(x+y,s)\Big| dydx \\
&\quad \le \int_0^n\int_{n-x}^\infty F(x,y)|Y(x+y,s)|dydx \\
&\quad = \int_0^n\int_n^\infty F(x,y-x)|Y(y,s)|dydx \\
&\quad = \int_n^\infty\int_0^n F(y-x,x)|Y(y,s)|dxdy \\
&\quad = \int_n^\infty\int_0^n F(x-y,y)|Y(x,s)|dydx \\
&\quad \le \int_n^\infty\int_0^x F(x-y,y)f_1(x,s)dydx + \int_n^\infty\int_0^x F(x-y,y)f_2(x,s)dydx \\
&\quad \le C\left[\int_n^\infty (1+x)f_1(x,s)dx + \int_n^\infty (1+x)f_2(x,s)dx\right] \qquad (3.27)
\end{aligned}$$

The right hand side of (3.27) is always bounded by the constant $C[\sup_{s\in[0,t]}\|f_1(s)\| + \sup_{s\in[0,t]}\|f_2(s)\|]$ and therefore

$$\int_0^t\int_0^n\int_{n-x}^\infty \Big|\mathrm{sgn}(Y(x,s))F(x,y)Y(x+y,s)\Big| dydxds = 0 \quad \text{as} \quad n\to\infty. \tag{3.28}$$

From (3.18), (3.20), (3.26) and (3.28) we can conclude that

$$\int_0^t S_4^n(s)ds \to 0 \quad as \quad n \to \infty.$$

The sequence u^n is bounded and monotone. Thus, from (3.15), (3.17) and (3.18) we obtain

$$\begin{aligned}
u(t) := \int_0^\infty (1+x)|Y(x,t)|dx = \lim_{n\to\infty} u^n(t) &\le \lim_{n\to\infty}\int_0^t \varphi(s)u^n(s)ds + \lim_{n\to\infty}\int_0^t S_4^n(s)ds \\
&= \int_0^t \varphi(s)\int_0^\infty (1+x)|Y(x,s)|dxds.
\end{aligned}$$

This gives the inequality

$$u(t) \le \int_0^t \varphi(s)u(s)ds$$

with $\varphi(s) \geq 0$. Then by Gronwall's inequality, we obtain

$$u(t) = \int_0^\infty (1+x)|Y(x,t)|dx = 0 \quad \text{for all} \quad t \in [0,T[.$$

Therefore,

$$f_1(x,t) = f_2(x,t) \quad \text{for a.e.} \quad x \in [0,\infty[.$$

□

Remarks. If we consider multiplicative coagulation kernel, i.e. $K(x,y) = kxy$ with the following much larger class of fragmentation kernels F

(H2"): There are constants $B_0 > 0$ and $\gamma > -1$ such that (3.5) holds.

Then the uniqueness of the solutions to (3.1)-(3.3) can be proved as in Theorem 3.2.4 by defining

$$u^n(t) := \int_0^n x|Y(x,t)|dx$$

and

$$f(x,y,t) = (x+y)\text{sgn}(Y(x+y,t)) - x\text{sgn}(Y(x,t)) - y\text{sgn}(Y(y,t)).$$

It should also be pointed out that (H2')(i) restricts the class of fragmentation kernels. It would be interesting to find a more general hypothesis on fragmentation kernels to replace (H2')(i) which could help us to prove uniqueness of solutions in X^+.

3.3 Uniqueness for the coagulation and multiple fragmentation equation

We refer the definition and the existence of solutions from chapter 2. The following further restrictions on the kernels are needed to prove the uniqueness of solutions to the coagulation equation with multiple fragmentation (2.1)-(2.2).

(HU1) $K(x,y)$ is a continuous non-negative function on $[0,\infty[\times[0,\infty[$ and Γ is a non-negative locally bounded function,

(HU2) K is symmetric, i.e. $K(x,y) = K(y,x)$ for all $x, y \in]0,\infty[$,

(HU3) $K(x,y) \leq \phi(x)\phi(y)$ for all x, y where $\phi(x) \leq k(1+x)^{\frac{1}{2}}$ for some constant k.

(HU4) for all $x > 0$, there exist m_1, $m_2 > 0$ such that

$$S(x) \leq m_1(1+x)^a$$

and

$$\int_0^x (1+y)^{\frac{1}{2}} b(y,x)dy \leq m_2(1+x)^b$$

where $a + b \leq \frac{1}{2}$.

Theorem 3.3.1. *If (HU1), (HU2), (HU3) and (HU4) hold and initial data $f_0 \in X^+$ then solutions to (2.1)-(2.2) are unique.*

Proof. Let f and g be two solutions to (2.1)-(2.2) on $[0, T[$ where $T > 0$, with $f(0) = g(0)$, and set $Y = f - g$. For $n = 1, 2, 3 \ldots$ we define

$$u^n(t) = \int_0^n (1+x)^{\frac{1}{2}} |Y(x,t)| dx.$$

Multiplying $|Y|$ by $(1+x)^{\frac{1}{2}}$ and applying Fubini's Theorem to Definition 2.1.2 (iv) above, we obtain for each n and $0 < t < T$,

$$\begin{aligned} u^n(t) = \int_0^t \int_0^n & (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) \\ & \times \left[\frac{1}{2} \int_0^x K(x-y,y)\{f(x-y,s)f(y,s) - g(x-y,s)g(y,s)\}dy \right. \\ & - \int_0^\infty K(x,y)\{f(x,s)f(y,s) - g(x,s)g(y,s)\}dy \\ & \left. + \int_x^\infty b(x,y)S(y)\{f(y,s) - g(y,s)\}dy - S(x)\{f(x,s) - g(x,s)\} \right] dxds. \end{aligned} \tag{3.29}$$

Using the substitution $x' = x - y$, $y' = y$ in the first integral on the right-hand side of (3.29) we find that

$$\begin{aligned} u^n(t) = \int_0^t \int_0^n \int_0^{n-x} & \left[\frac{1}{2}(1+x+y)^{\frac{1}{2}} \mathrm{sgn}(Y(x+y,s)) - (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) \right] \\ & \times K(x,y)\{f(x,s)f(y,s) - g(x,s)g(y,s)\}dydxds \\ - \int_0^t \int_0^n \int_{n-x}^\infty & (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) \\ & \times K(x,y)\{f(x,s)f(y,s) - g(x,s)g(y,s)\}dydxds \\ + \int_0^t \int_0^n \int_x^\infty & (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) b(x,y)S(y)\{f(y,s) - g(y,s)\}dydxds \\ - \int_0^t \int_0^n & (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s))S(x)\{f(x,s) - g(x,s)\}dxds. \end{aligned} \tag{3.30}$$

By interchanging the order of integration and interchanging the roles of x and y, the symmetry of K yields the identity

$$\begin{aligned}
&\int_0^n \int_0^{n-x} (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) K(x,y) \{f(x,s)f(y,s) - g(x,s)g(y,s)\} dydx \\
&\quad = \int_0^n \int_0^{n-x} (1+y)^{\frac{1}{2}} \mathrm{sgn}(Y(y,s)) K(x,y) \{f(x,s)f(y,s) - g(x,s)g(y,s)\} dydx. \qquad (3.31)
\end{aligned}$$

For $x, y > 0$ and $t \in [0, T[$ we define the function r by

$$r(x,y,t) = (1+x+y)^{\frac{1}{2}} \mathrm{sgn}(Y(x+y,t)) - (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,t)) - (1+y)^{\frac{1}{2}} \mathrm{sgn}(Y(y,t)).$$

Using (3.31) we can show that (3.30) can be rewritten as

$$\begin{aligned}
u^n(t) = &\frac{1}{2} \int_0^t \int_0^n \int_0^{n-x} r(x,y,s) K(x,y) f(x,s) Y(y,s) dydxds \\
&+ \frac{1}{2} \int_0^t \int_0^n \int_0^{n-x} r(x,y,s) K(x,y) g(y,s) Y(x,s) dydxds \\
&+ \int_0^t \int_0^n \int_x^\infty (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) b(x,y) S(y) Y(y,s) dydxds \\
&- \int_0^t \int_0^n (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) S(x) Y(x,s) dxds \\
&- \int_0^t \int_0^n \int_{n-x}^\infty (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) \\
&\qquad \times K(x,y) \{f(x,s)Y(y,s) + g(y,s)Y(x,s)\} dydxds. \qquad (3.32)
\end{aligned}$$

Since the fourth integral and the last term in the fifth integral on the right-hand side of (3.32) are non-negative. We may omit them. Thus we obtain, by interchanging the order of integration for the third integral,

$$\begin{aligned}
u^n(t) \leq &\frac{1}{2} \int_0^t \int_0^n \int_0^{n-x} r(x,y,s) K(x,y) f(x,s) Y(y,s) dydxds \\
&+ \frac{1}{2} \int_0^t \int_0^n \int_0^{n-x} r(x,y,s) K(x,y) g(y,s) Y(x,s) dydxds \\
&+ \int_0^t \int_0^n \int_0^y (1+x)^{\frac{1}{2}} b(x,y) S(y) |Y(y,s)| dxdyds \\
&+ \int_0^t \int_0^n \int_n^\infty (1+x)^{\frac{1}{2}} b(x,y) S(y) |Y(y,s)| dydxds \\
&- \int_0^t \int_0^n \int_{n-x}^\infty (1+x)^{\frac{1}{2}} \mathrm{sgn}(Y(x,s)) K(x,y) f(x,s) Y(y,s) dydxds \\
=: &\int_0^t \sum_{i=1}^5 S_i^n(s) ds. \qquad (3.33)
\end{aligned}$$

Here S_i^n, for $i = 1, \dots 5$, are the corresponding integrands in the preceding lines.

We now consider each S_i^n individually. Note that for all $q, q_1, q_2 \in \mathbb{R}$, we have

$$\mathrm{sgn}(q_1)\mathrm{sgn}(q_2) = \mathrm{sgn}(q_1 q_2) \quad \text{and} \quad |q| = q\mathrm{sgn}(q).$$

We find that

$$\begin{aligned} r(x,y,s)Y(y,s) &\leq [(1+x+y)^{\frac{1}{2}} + (1+x)^{\frac{1}{2}} - (1+y)^{\frac{1}{2}}]|Y(y,s)| \\ &\leq [(1+x)^{\frac{1}{2}} + (1+y)^{\frac{1}{2}} + (1+x)^{\frac{1}{2}} - (1+y)^{\frac{1}{2}}]|Y(y,s)| \\ &\leq 2(1+x)^{\frac{1}{2}}|Y(y,s)|. \end{aligned} \tag{3.34}$$

Now, by using (HU3) we consider

$$\begin{aligned} \int_0^t S_1^n(s)ds &= \frac{1}{2}\int_0^t \int_0^n \int_0^{n-x} r(x,y,s)K(x,y)f(x,s)Y(y,s)dydxds \\ &\leq \int_0^t \int_0^n \int_0^{n-x} (1+x)^{\frac{1}{2}} K(x,y)f(x,s)|Y(y,s)|dydxds \\ &\leq k^2 \int_0^t \int_0^n \int_0^{n-x} (1+x)(1+y)^{\frac{1}{2}} f(x,s)|Y(y,s)|dydxds \\ &\leq R_1 \int_0^t u^n(s)ds, \quad \text{where} \quad R_1 = k^2 \sup_{s\in[0,t]} \|f(s)\|. \end{aligned} \tag{3.35}$$

Similarly, there is a constant R_2 such that

$$\int_0^t S_2^n(s)ds \leq R_2 \int_0^t u^n(s)ds. \tag{3.36}$$

Now, we consider

$$\int_0^t S_3^n(s)ds = \int_0^t \int_0^n \int_0^y (1+x)^{\frac{1}{2}} b(x,y)S(y)|Y(y,s)|dxdyds. \tag{3.37}$$

By interchanging the role of x and y in (3.37) and using (HU4) we obtain

$$\begin{aligned} \int_0^t S_3^n(s)ds &= \int_0^t \int_0^n \int_0^x (1+y)^{\frac{1}{2}} b(y,x)S(x)|Y(x,s)|dydxds \\ &\leq m_1 m_2 \int_0^t \int_0^n (1+x)^{a+b}|Y(x,s)|dxds \\ &\leq R_3 \int_0^t u^n(s)ds, \quad \text{where} \quad R_3 = m_1 m_2. \end{aligned} \tag{3.38}$$

Next, using Fubini's theorem and hypothesis (HU4) we have for each $s \in [0,t]$

$$\begin{aligned}\int_0^n \int_n^\infty (1+x)^{\frac{1}{2}} b(x,y)S(y)|Y(y,s)|dydx \\ &= \int_n^\infty \int_0^n (1+y)^{\frac{1}{2}} b(y,x)S(x)|Y(x,s)|dydx \\ &\leq \int_n^\infty \int_0^x (1+y)^{\frac{1}{2}} b(y,x)S(x)[f(x,s)+g(x,s)]dydx \\ &\leq m_1 m_2 \int_n^\infty (1+x)^{a+b}[f(x,s)+g(x,s)]dydx. \end{aligned} \tag{3.39}$$

The right-hand side of (3.39) is always bounded by the constant $m_1 m_2 \sup_{s\in[0,t]}[\|f(s)\| + \|g(s)\|]$ and therefore the dominated convergence theorem leads to

$$\int_0^t S_4^n(s)ds \to 0 \quad \text{as} \quad n \to \infty. \tag{3.40}$$

To consider S_5^n we first observe that

$$\begin{aligned}\left| \int_0^\infty \int_0^\infty (1+x)^{\frac{1}{2}} \operatorname{sgn}(Y(x,s))K(x,y)f(x,s)Y(y,s)dydx \right| \\ &\leq k^2 \int_0^\infty \int_0^\infty (1+x)(1+y)^{\frac{1}{2}} f(x,s)|Y(y,s)|dydx \\ &< \infty. \end{aligned}$$

Thus, from Lemma 3.1.2 we find that

$$\int_0^t S_5^n(s)ds \to 0 \quad \text{as} \quad n \to \infty. \tag{3.41}$$

The sequence u^n is bounded and monotone. Thus, from (3.33), (3.35), (3.36), (3.38), (3.40), (3.41) and taking $R = R_1 + R_2 + R_3$ we obtain

$$\begin{aligned} u(t) := \int_0^\infty (1+x)^{\frac{1}{2}}|Y(x,t)|dx &= \lim_{n\to\infty} u^n(t) \\ &\leq \lim_{n\to\infty} \int_0^t \sum_{i=1}^5 S_i^n(s)ds \\ &\leq \lim_{n\to\infty} R \int_0^t u^n(s)ds + \lim_{n\to\infty} \int_0^t [S_4^n(s) + S_5^n(s)]ds \\ &= R \int_0^t \int_0^\infty (1+x)^{\frac{1}{2}}|Y(x,s)|dxds. \end{aligned}$$

This gives the inequality

$$u(t) \leq R \int_0^t u(s)ds. \tag{3.42}$$

Then by applying Gronwall's inequality to (3.42), we obtain

$$u(t) = \int_0^\infty (1+x)^{\frac{1}{2}} |Y(x,t)| dx = 0 \quad \text{for all} \quad t \in [0, T[.$$

Therefore, we obtain

$$f(x,t) = g(x,t) \quad \text{for a.e.} \quad x \in]0, \infty[.$$

□

Chapter 4

An extension of existence theory

The purpose of this chapter is to study the existence of solutions to the continuous coagulation equation with multiple fragmentation that includes some classical multiple fragmentation kernels that are not covered in Chapter 2. Here we consider the same classes of coagulation kernels as are in Chapter 2. This is an extension of results studied in Chapter 2 and Giri et al. [40]. The existence of solutions is also proved in the same space as is in Chapter 2.

We now organize the content of this chapter. For the completeness, a short description of the continuous coagulation and multiple fragmentation equation from Chapter 1 is again reviewed in the next section. In Section 4.1, we repeat some definitions of norm and solutions from Chapter 2 and make some hypotheses on kernels which play an important role in further analysis. In Section 4.2, we obtain a sequence of unique global solutions truncated equations to (4.1)-(4.2) and extract a weakly convergent subsequence in L^1. Finally, we show that the limit function obtained from weakly convergent subsequence is actually a solution to (4.1)-(4.2).

4.1 Introduction

The non-linear continuous coagulation and multiple fragmentation equation is given by

$$\frac{\partial f(x,t)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)f(x-y,t)f(y,t)dy - \int_0^\infty K(x,y)f(x,t)f(y,t)dy + \int_x^\infty b(x,y)S(y)f(y,t)dy - S(x)f(x,t), \tag{4.1}$$

with

$$f(x,0) = f_0(x) \geq 0 \quad a.e. \tag{4.2}$$

Here $f(x,t)$ denote the number density of particles of size $x \geq 0$ at time $t \geq 0$. The interpretation for coagulation and fragmentation terms can be followed from Chapter 2.

We also repeat the definition of the selection function S and breakage function b in terms of the multiple-fragmentation kernel Γ which are as follows

$$S(x) = \int_0^x \frac{y}{x}\Gamma(x,y)dy, \qquad b(x,y) = \Gamma(y,x)/S(y). \tag{4.3}$$

The breakage function has the following properties

$$\int_0^y b(x,y)dx = N < \infty, \quad \text{for all} \quad y > 0 \quad \text{and} \qquad b(x,y) = 0, \quad \text{for} \quad x > y, \tag{4.4}$$

and

$$\int_0^y xb(x,y)dx = y \quad \text{for all} \quad y > 0. \tag{4.5}$$

The above properties can be found with more details in Chapter 2. The main novelty of the result is that it includes some classical multiple-fragmentation kernels which are not considered in Chapter 2. The examples of such fragmentation kernels are given at the end of this section. The classes of coagulation kernels are same as in Chapter 2. In order to prove the existence of solutions to (4.1)-(4.2), we define the following Banach space X with norm $\|\cdot\|$

$$X = \{f \in L^1(0,\infty) : \|f\| < \infty\} \quad \text{where} \quad \|f\| = \int_0^\infty (1+x)|f(x)|dx.$$

We also take again the norms

$$\|f\|_x = \int_0^\infty x|f(x)|dx \quad \text{and} \quad \|f\|_1 = \int_0^\infty |f(x)|dx$$

and set

$$X^+ = \{f \in X : f \geq 0 \quad a.e.\}.$$

Let us make the following hypotheses on the coagulation kernels K, multiple-fragmentation kernel Γ and selection rate S which will be used in the further analysis

Hypotheses 4.1.1. *(H1) K is a continuous non-negative function on* $[0,\infty[\times[0,\infty[$,

(H2) K is symmetric, i.e. $K(x,y) = K(y,x)$ for all $x,y \in]0,\infty[$,

(H3) $K(x,y) \leq \phi(x)\phi(y)$ for all $x,y \in]0,\infty[$ where $\phi(x) \leq k_1(1+x)^\mu$ for some $0 \leq \mu < 1$ and constant k_1.

For each $R \geq 1$, we have

(H4) for $R < y$ the estimate $\Gamma(y,x) \leq k(R)y^{\theta}$, $0 < x < R < y$ for some $\theta \in [0,1[$,

(H5) for $R \geq y$ we define for any set $E \subset \mathbb{R}_{>0}$ the indicator function $\mathbb{1}_E$ with

$$\mathbb{1}_E(x) := \begin{cases} 1 & \text{if } x \in E, \\ 0 & \text{if } x \notin E, \end{cases}$$

and assume the estimates

$$\int_0^y \mathbb{1}_E(x)\Gamma(y,x)dx \leq \omega(R,|E|), \quad y \in]0,R],$$

with

$$\lim_{\delta \to 0} \omega(R,\delta) = 0,$$

where E is any measurable subset of $]0,R]$ with $|E| \leq \delta$,

(H6) $S \in L^{\infty}]0,R[$.

Definition 4.1.2. *Let $T \in]0,\infty]$. A solution f of (4.1-4.2) is a function $f : [0,T[\to X^+$ such that for a.e. $x \in]0,\infty[$ and all $t \in [0,T[$ the following hold*

(i) $f(x,t) \geq 0$,

(ii) $f(x,.)$ is continuous on $[0,T[$,

(iii) the following integrals are bounded

$$\int_0^t \int_0^{\infty} K(x,y)f(y,s)dyds < \infty \quad \text{and} \quad \int_0^t \int_x^{\infty} b(x,y)S(y)f(y,s)dyds < \infty,$$

(iv) the function f satisfies the following weak formulation of (4.1)

$$\begin{aligned} f(x,t) = f_0(x) + \int_0^t \Bigg\{ \frac{1}{2} \int_0^x K(x-y,y)f(x-y,s)f(y,s)dy \\ - \int_0^{\infty} K(x,y)f(x,s)f(y,s)dy + \int_x^{\infty} b(x,y)S(y)f(y,s)dy - S(x)f(x,s) \Bigg\} ds. \end{aligned}$$

The examples of coagulation kernels which satisfy the growth conditions in hypotheses 4.1.1 are the same as in Chapter 2. Let us now take the following types of fragmentation kernels which also fit in the classes considered in Hypotheses 4.1.1. If we assume that

$$\Gamma = S \cdot b \in L^{\infty}(]0,\infty[\times]0,\infty[),$$

then these kernels have been analyzed in McLaughlin et al. [66] and Chapter 2 also. Now let us take the examples of type

$$S(y) = y^{\gamma} \quad \text{and} \quad b(x,y) = \frac{\alpha+2}{y}\left(\frac{x}{y}\right)^{\alpha}, \quad \text{for} \quad 0 < x < y,$$

where $\gamma > 0$ and $\alpha \geq 0$. These have been studied in Peterson [77] and also in Ziff [102]. Then, we have

$$\Gamma(y,x) = (\alpha+2)x^{\alpha}y^{\gamma-(\alpha+1)}.$$

Using Hölder's inequality one obtains

$$\begin{aligned}
\int_0^y \mathbb{1}_E(x)\Gamma(y,x)dx &= (\alpha+2)y^{\gamma-(\alpha+1)}\int_0^y \mathbb{1}_E(x)x^{\alpha}dx \\
&\leq (\alpha+2)y^{\gamma-(\alpha+1)}|E|^{\frac{\gamma}{\gamma+1}}\left(\int_0^y x^{\alpha(\gamma+1)}dx\right)^{\frac{1}{\gamma+1}} \\
&\leq (\alpha+2)|E|^{\frac{\gamma}{\gamma+1}}(1+\alpha(\gamma+1))^{-\frac{1}{\gamma+1}}y^{\alpha+\frac{1}{\gamma+1}+\gamma-(\alpha+1)} \\
&\leq C(\alpha,\gamma)y^{\frac{\gamma^2}{\gamma+1}}|E|^{\frac{\gamma}{\gamma+1}} \\
&\leq C(\alpha,\gamma)R^{\frac{\gamma^2}{\gamma+1}}|E|^{\frac{\gamma}{\gamma+1}}.
\end{aligned}$$

This shows that (H5) is fulfilled. As for (H4), we can write

$$\Gamma(y,x) \leq (\alpha+2)y^{\gamma-1} \leq \frac{\alpha+2}{R^{1+\theta-\gamma}}y^{\theta}$$

provided $\gamma < 1+\theta$ for some $\theta \in [0,1[$. Thus (H4) is satisfied for $\gamma < 2$. This shows that these type of fragmentation kernels satisfy the hypotheses mentioned above but are not included in Chapter 2.

4.2 Existence

4.2.1 Approximating equations

In order to prove the existence of solutions to (4.1-4.2), we take the limit of a sequence of approximating equations obtained by replacing the kernel K and selection function S by the 'cut-off' kernels K_n and S_n as in Chapter 2, where

$$K_n(x,y) := \begin{cases} K(x,y) & \text{if } x+y < n, \\ 0 & \text{if } x+y \geq n, \end{cases}$$

$$S_n(x) := \begin{cases} S(x) & \text{if } 0 < x < n, \\ 0 & \text{if } x \geq n. \end{cases}$$

The approximating equations, with solutions denoted by f^n, are written as

$$\begin{aligned} \frac{\partial f^n(x,t)}{\partial t} =& \frac{1}{2}\int_0^x K_n(x-y,y)f^n(x-y,t)f^n(y,t)dy - \int_0^{n-x} K_n(x,y)f^n(x,t)f^n(y,t)dy \\ &+ \int_x^n b(x,y)S_n(y)f^n(y,t)dy - S_n(x)f^n(x,t), \end{aligned} \tag{4.6}$$

with

$$f_0^n(x) := \begin{cases} f_0(x) & \text{if } 0 < x < n, \\ 0 & \text{if } x \geq n. \end{cases} \tag{4.7}$$

Choose $T > 0$. We may argue as in Stewart [89, Theorem 3.1] and obtain the following result. For each $n = 1, 2, 3, \ldots$, (4.6-4.7) has a unique solution $f^n \in X^+$ with $f^n(x,t) \geq 0$ for a.e. $x \in]0, n[$ and $t \in [0, \infty[$, see Walker [98] also. Moreover, the total mass remains conserved, for all $t \in [0, \infty[$, i.e.

$$\int_0^n x f^n(x,t)dx = \int_0^n x f_0^n(x)dx. \tag{4.8}$$

From now on we consider the 'zero extension' of each f^n on $\mathbb{R}$, i.e.

$$\widehat{f^n}(x,t) := \begin{cases} f^n(x,t) & \text{if } 0 < x < n, \quad t \in [0,T] \\ 0 & \text{if } x \leq 0 \quad or \quad x \geq n. \end{cases}$$

For the simplicity we drop the $\widehat{\cdot}$ notation for the remainder of the work and the subscripts on the coagulation kernels and the selection functions.

Next, we need to prove the following lemma to apply the *Dunford-Pettis-Theorem* [23, Theorem 4.21.2] and then equicontinuity of the sequence $(f^n)_{n\in\mathbb{N}}$ in time to use the *Arzelà-Ascoli Theorem* [3, Appendix A8.5].

Lemma 4.2.1. *Assume that (H1), (H2), (H3), (H4), (H5) and (H6) hold. Then the following results are true:*

$$(i) \quad \int_0^\infty (1+x)f^n(x,t)dx \leq L \quad for \quad n = 1, 2, 3\ldots \quad and\ all \quad t \in [0,T],$$

(ii) For any $\epsilon > 0$ there exists an $R > 0$ such that for all $t \in [0,T]$

$$\sup_n \left\{ \int_R^\infty f^n(x,t)dx \right\} \leq \epsilon,$$

(iii) given $\epsilon > 0$ there exists a $\delta > 0$ such that for every measurable set E with $|E| \leq \delta$ and for all $n = 1, 2, 3\dots$ with $t \in [0, T]$

$$\int_E f^n(x,t)dx < \epsilon.$$

Proof. (i) By integrating (4.6) with respect to x and t, then using Fubini's Theorem, for each $n \geq 1$ we have

$$\begin{aligned}\int_0^1 f^n(x,t)dx =& -\frac{1}{2}\int_0^t\int_0^1\int_0^{1-x} K(x,y)f^n(x,s)f^n(y,s)dydxds \\ &- \int_0^t\int_0^1\int_{1-x}^{n-x} K(x,y)f^n(x,s)f^n(y,s)dydxds \\ &+ \int_0^t\int_0^1\int_x^n b(x,y)S(y)f^n(y,s)dydxds - \int_0^t\int_0^1 S(x)f^n(x,s)dxds \\ &+ \int_0^1 f^n(x,0)dx.\end{aligned}$$

Since the integrands are all non-negative, we may estimate

$$\begin{aligned}\int_0^1 f^n(x,t)dx \leq& \int_0^t\int_0^1\int_x^n b(x,y)S(y)f^n(y,s)dydxds + \int_0^1 f^n(x,0)dx \\ =& \int_0^t\int_0^1\int_x^1 b(x,y)S(y)f^n(y,s)dydxds \\ &+ \int_0^t\int_0^1\int_1^n b(x,y)S(y)f^n(y,s)dydxds + \int_0^1 f^n(x,0)dx.\end{aligned}$$

We use Fubini's Theorem in the first term on the right hand side to get

$$\begin{aligned}\int_0^1 f^n(x,t)dx \leq& \int_0^t\int_0^1 f^n(y,s)\int_0^y b(x,y)S(y)dxdyds \\ &+ \int_0^t\int_0^1\int_1^n b(x,y)S(y)f^n(y,s)dydxds + \int_0^1 f^n(x,0)dx \\ \leq& \int_0^t\int_0^1 f^n(y,s)\int_0^y \mathbb{1}_{]0,1[}(x)\Gamma(y,x)dxdyds \\ &+ \int_0^t\int_0^1\int_1^n \Gamma(y,x)f^n(y,s)dydxds + \int_0^1 f^n(x,0)dx.\end{aligned}$$

Using (H5) and (H4) in the first and second terms on the right hand side respectively, we obtain

$$\begin{aligned}\int_0^1 f^n(x,t)dx \leq &\omega(1,1)\int_0^t\int_0^1 f^n(y,s)dyds \\ &+ k(1)\int_0^t\int_0^1\int_1^n yf^n(y,s)dydxds + \int_0^1 f^n(x,0)dx \\ \leq &\omega(1,1)\int_0^t\int_0^1 f^n(y,s)dyds \\ &+ k(1)\int_0^t\int_1^n yf^n(y,s)dyds + \int_0^1 f^n(x,0)dx\end{aligned} \tag{4.9}$$

From equation (4.8), for $s \in [0,T]$

$$\|f^n(s)\|_x = \|f^n(0)\|_x \leq \|f(0)\|. \tag{4.10}$$

Using (4.9) and (4.10) we obtain

$$\begin{aligned}\int_0^1 f^n(x,t)dx &\leq \omega(1,1)\int_0^t\int_0^1 f^n(y,s)dyds + k(1)T\|f_0\| + \|f_0\| \\ &= \omega(1,1)\int_0^t\int_0^1 f^n(y,s)dyds + \|f_0\|(k(1)T+1).\end{aligned}$$

Applying Gronwall's Lemma, see e.g. Walter [99, p. 310], we obtain

$$\int_0^1 f^n(x,t)dx \leq \|f_0\|(k(1)T+1)\exp(\omega(1,1)T).$$

Thus, by using (4.8) again we may estimate

$$\begin{aligned}\int_0^\infty (1+x)f^n(x,t)dx &= \int_0^1 f^n(x,t)dx + \int_1^n f^n(x,t)dx + \int_0^n xf^n(x,t)dx \\ &\leq \int_0^1 f^n(x,t)dx + \int_1^n xf^n(x,t)dx + \|f_0\| \\ &\leq \|f_0\|[(k(1)T+1)\exp(\omega(1,1)T)+2] =: L.\end{aligned}$$

(ii) For $\epsilon > 0$, let $R > 0$ be such that $R > \|f_0\|/\epsilon$. Then, by (4.10), for each $n = 1, 2, 3, \ldots$ and for all $t \in [0,T]$ we have

$$\begin{aligned}\int_R^\infty f^n(x,t)dx &= \int_R^\infty (x/x)f^n(x,t)dx \\ &\leq \frac{1}{R}\int_R^\infty xf^n(x,t)dx \leq \frac{1}{R}\|f_0\| < \epsilon.\end{aligned}$$

(iii) Let us consider a measurable subset $E \subset]0,R[$ with $|E| \leq \delta$. For $n = 1, 2, 3, \ldots$ and $t \in [0,T]$, we define

$$p^n(\delta, t) = \sup\left\{ \int_0^R \mathbb{1}_E(x) f^n(x,t)dx : E \subset]0,R[\ \text{ and } \ |E| \leq \delta \right\}.$$

Using the non-negativity of each f^n and (4.6)-(4.7), we have

$$\begin{aligned}
&\int_0^R \mathbb{1}_E(x) f^n(x,t)dx \\
&\qquad \leq \frac{1}{2}\int_0^t \int_0^R \mathbb{1}_E(x) \int_0^x K(x-y,y) f^n(x-y,s) f^n(y,s)dydxds \\
&\qquad\quad + \int_0^t \int_0^R \mathbb{1}_E(x) \int_x^\infty b(x,y)S(y) f^n(y,s)dydxds + p^n(\delta,0).
\end{aligned}$$

Application of Fubini's Theorem to the first and second integrals on the right hand side gives us

$$\begin{aligned}
&\int_0^R \mathbb{1}_E(x) f^n(x,t)dx \\
&\qquad \leq \frac{1}{2}\int_0^t \int_0^R f^n(y,s) \int_y^R \mathbb{1}_E(x) K(y,x-y) f^n(x-y,s)dxdyds \\
&\qquad\quad + \int_0^t \int_0^R f^n(y,s) \int_0^y \mathbb{1}_E(x) \Gamma(y,x)dxdyds \\
&\qquad\quad + \int_0^t \int_0^R \mathbb{1}_E(x) \int_R^\infty \Gamma(y,x) f^n(y,s)dydxds + p^n(\delta,0).
\end{aligned}$$

Using the substitution $x' = x - y$, $y' = y$ in the first integral, we obtain

$$\begin{aligned}
&\int_0^R \mathbb{1}_E(x) f^n(x,t)dx \\
&\qquad \leq \frac{1}{2}\int_0^t \int_0^R f^n(y,s) \int_0^{R-y} \mathbb{1}_E(x+y) K(y,x) f^n(x,s)dxdyds \\
&\qquad\quad + \int_0^t \int_0^R f^n(y,s) \int_0^y \mathbb{1}_E(x) \Gamma(y,x)dxdyds \\
&\qquad\quad + \int_0^t \int_0^R \mathbb{1}_E(x) \int_R^\infty \Gamma(y,x) f^n(y,s)dydxds + p^n(\delta,0).
\end{aligned}$$

For some $y \in \mathbb{R}_{>0}$ we denote by $y + E$ the set

$$\{z \in \mathbb{R}_{>0} : z = y + x \ \text{ for some } \ x \in E\}.$$

We use (H3), (H5) and (H4) in first, second and third integrals on the right-hand side respectively to get

$$\begin{aligned}\int_0^R &\mathbb{1}_E(x) f^n(x,t)dx \\ &\leq \frac{k_1^2}{2}(1+R)^\mu \int_0^t \int_0^R (1+y)^\mu f^n(y,s)dy \int_0^R f^n(x,s)\mathbb{1}_{-y+E\bigcap[0,R-y]}(x)dxds \\ &\quad + \omega(R,|E|)\int_0^t \int_0^R f^n(y,s)dyds \\ &\quad + k(R)\int_0^t \int_0^\infty y f^n(y,s)dyds \cdot \int_0^R \mathbb{1}_E(x)dx + p^n(\delta,0).\end{aligned}$$

By using Lemma 4.2.1(i), this can be rewritten as

$$\begin{aligned}\int_0^R \mathbb{1}_E(x) f^n(x,t)dx \leq &\frac{k_1^2}{2}(1+R)^\mu L \int_0^t \int_0^R f^n(x,s)\mathbb{1}_{-y+E\bigcap[0,R-y]}(x)dxds \\ &+ LT[\omega(R,|E|) + k(R)|E|] + p^n(\delta,0).\end{aligned} \tag{4.11}$$

Since

$$-y + E\cap]0,R-y[= \{x \in [0,R], \quad 0 < x < R-y, \quad x+y \in E\}.$$

Then, we have

$$\left| -y + E\cap]0,R-y[\right| = \int_0^{R-y} \mathbb{1}_{-y+E}(x)dx = \int_y^R \mathbb{1}_E(x)dx \leq |E|. \tag{4.12}$$

By using (4.12), the definition of $p^n(\delta,t)$, and a suitable constant $C(R) > 0$ (4.11) can be further rewritten as

$$\int_0^R \mathbb{1}_E(x) f^n(x,t)dx \leq C(R)\int_0^t p^n(\delta,s)ds + LT[\omega(R,\delta) + k(R)\delta] + p^n(\delta,0).$$

Taking the supremum over all E such that $E \subset]0,R[$ with $|E| \leq \delta$ gives

$$p^n(\delta,t) \leq p^n(\delta,0) + LT[\omega(R,\delta) + k(R)\delta] + C(R)\int_0^t p^n(\delta,s)ds.$$

By using Gronwall's inequality, see e.g. Walter [99, p. 310], we obtain

$$p^n(E,t) \leq [p^n(\delta,0) + LT\{\omega(R,\delta) + k(R)\delta\}] \exp\{C(R)t\}. \tag{4.13}$$

By (4.13), we obtain for $n = 1,2,3,\ldots$ and $t \in [0,T]$

$$\begin{aligned}\int_E f^n(x,t)dx = &\int_0^R \mathbb{1}_E(x) f^n(x,t)dx \\ &\leq p^n(\delta,t) \\ &\leq [p^n(\delta,0) + LT\{\omega(R,\delta) + k(R)\delta\}] \exp\{C(R)t\}.\end{aligned}$$

Due to the absolute continuity of the integral we have $p^n(\delta, 0) \to 0$ for $\delta \to 0$. This implies that

$$\int_E f^n(x,t)dx \to 0 \quad \text{as} \quad \delta \to 0.$$

$\square$

The above Lemma 4.2.1 implies that for each $t \in [0,T]$, the sequence of functions $(f^n(t))_{n\in\mathbb{N}}$ lies in a weakly relatively compact set in $L^1]0,\infty[$ by the *Dunford-Pettis-Theorem.*

4.2.2 Equicontinuity in time

Now we proceed in this section to show equicontinuity of the sequence $(f^n)_{n\in\mathbb{N}}$ in time. In this section, the part of coagulation terms will be the same as in Chapter 2. For the completeness, we repeat that also. Choose $\epsilon > 0$ and $\phi \in L^\infty]0,\infty[$. Let $s,t \in [0,T]$ and assume $t \geq s$. Choose $R > 1$ such that

$$\|\phi\|_{L^\infty} 2L/R < \epsilon/2. \tag{4.14}$$

For each n, by Lemma 4.2.1(i),

$$\int_R^\infty |f^n(x,t) - f^n(x,s)|dx \leq \frac{1}{R}\int_R^\infty x\{f^n(x,t) + f^n(x,s)\}dx \leq 2L/R. \tag{4.15}$$

By using (4.6), (4.14) and (4.15), we get using $t \geq s$

$$\begin{aligned}
\left|\int_0^\infty \phi(x)\{f^n(x,t) - f^n(x,s)\}dx\right| \\
\leq & \left|\int_0^R \phi(x)\{f^n(x,t) - f^n(x,s)\}dx\right| \\
& + \int_R^\infty |\phi(x)|\{|f^n(x,t) - f^n(x,s)|\}dx \\
\leq & \|\phi\|_{L^\infty]0,\infty[} \int_s^t \left[\frac{1}{2}\int_0^R \int_0^x K(x-y,y)f^n(x-y,\tau)f^n(y,\tau)dydx\right. \\
& + \int_0^R \int_0^{n-x} K(x,y)f^n(x,\tau)f^n(y,\tau)dydx \\
& + \int_0^R \int_x^n b(x,y)S(y)f^n(y,\tau)dydx \\
& \left. + \int_0^R S(x)f^n(x,\tau)dx\right]d\tau + \epsilon/2.
\end{aligned} \tag{4.16}$$

Now we consider the first term on the right hand side of (4.16), by Fubini's Theorem, (H1)-(H3) and Lemma 4.2.1 (i), we have

$$\begin{aligned}
&\frac{1}{2}\int_0^R \int_0^x K(x-y,y)f^n(x-y,\tau)f^n(y,\tau)dydx \\
&\qquad = \frac{1}{2}\int_0^R \int_y^m K(x-y,y)f^n(x-y,\tau)f^n(y,\tau)dxdy \\
&\qquad = \frac{1}{2}\int_0^R \int_0^{m-y} K(x,y)f^n(x,\tau)f^n(y,\tau)dxdy \\
&\qquad = \frac{1}{2}\int_0^R \int_0^{m-x} K(y,x)f^n(y,\tau)f^n(x,\tau)dydx \\
&\qquad = \frac{1}{2}\int_0^R \int_0^{m-x} K(x,y)f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \leq k_1^2\frac{1}{2}\int_0^R \int_0^{m-x} (1+x)^\mu(1+y)^\mu f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \leq \frac{1}{2}k_1^2L^2.
\end{aligned}$$

Similarly, for the second term we may estimate

$$\begin{aligned}
&\int_0^R \int_0^{n-x} K(x,y)f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \leq k_1^2\int_0^R \int_0^{n-x} (1+x)^\mu(1+y)^\mu f^n(x,\tau)f^n(y,\tau)dydx \\
&\qquad \leq k_1^2L^2.
\end{aligned}$$

For $n > R$, the third term using (H4), (H5) and Lemma 4.2.1 (i) gives that

$$\begin{aligned}
&\int_0^R \int_x^n b(x,y)S(y)f^n(y,\tau)dydx \\
&\quad =\int_0^R \int_0^y \Gamma(y,x)f^n(y,\tau)dxdy + \int_0^R \int_R^\infty \Gamma(y,x)f^n(y,\tau)dydx \\
&\quad \leq \int_0^R f^n(y,\tau)\int_0^y \mathbb{1}_{]0,R[}(x)\Gamma(y,x)dxdy + \int_0^R \int_R^\infty \Gamma(y,x)f^n(y,\tau)dydx \\
&\quad \leq \omega(R,R)\int_0^R f^n(y,\tau)dy + k(R)\int_0^R \int_R^\infty yf^n(y,\tau)dydx \\
&\quad \leq [\omega(R,R) + Rk(R)]L.
\end{aligned}$$

Similarly we can obtain the above inequality for $R > n$ though this is not needed here. For the fourth term, by using (H6) and Lemma 4.2.1 (i) we have

$$\int_0^R S(x)f^n(x,t)dx \leq \|S\|_{L^\infty]0,R[}L.$$

By using the above inequalities, the equation (4.16) reduces to

$$\left| \int_0^\infty \phi(x)\{f^n(x,t) - f^n(x,s)\}dx \right|$$
$$\leq \|\phi\|_{L^\infty]0,\infty[}(t-s)\left[\frac{3}{2}k_1^2 L^2 + \{\omega(R,R) + k'(R) + \|S\|_{L^\infty]0,R[}\}L\right] + \epsilon/2 < \epsilon \tag{4.17}$$

whenever $t - s < \delta$ for some suitable $\delta > 0$. The argument given above similarly holds if $s > t$. Hence (4.17) is true for all n and $|t - s| < \delta$. This implies the time equicontinuity of the family $\{f^n(t), t \in [0,T]\}$ in $L^1(\mathbb{R}_{>0})$. Thus, $\{f^n(t), t \in [0,T]\}$ lies in a relatively compact subset of the *gauge space* Ω. So, we may apply refined version of *Arzelà-Ascoli Theorem*, see [89, Theorem 2.1] to conclude that there exists a subsequence f^{n_k} such that

$$f^{n_k}(t) \to f(t) \ \text{ in } \ \Omega \ \text{ as } \ n_k \to \infty$$

uniformly for $t \in [0,T]$ and for some $f \in C([0,T];\Omega)$.

4.2.3 Passing to the limit

Similar to Chapter 2, we suppress the dependence on arbitrary but fixed $t \in [0,T]$ when it is not explicitly needed. Now we have to show that the limit function which we obtained above is actually a solution to (4.1-4.2). Define the operators Q_i^n, Q_i, $i = 1$ to 4, to be

$$Q_1^n(f^n)(x) = \frac{1}{2}\int_0^x K(x-y,y)f^n(x-y)f^n(y)dy,$$
$$Q_1(f)(x) = \frac{1}{2}\int_0^x K(x-y,y)f(x-y)f(y)dy,$$
$$Q_2^n(f^n)(x) = \int_0^{n-x} K(x,y)f^n(x)f^n(y)dy, \qquad Q_2(f)(x) = \int_0^\infty K(x,y)f(x)f(y)dy,$$
$$Q_3^n(f^n)(x) = S(x)f^n(x), \qquad Q_3(f)(x) = S(x)f(x),$$
$$Q_4^n(f^n)(x) = \int_x^n b(x,y)S(y)f^n(y)dy, \qquad Q_4(f)(x) = \int_x^\infty b(x,y)S(y)f(y)dy,$$

where $f \in L^1]0,\infty[$, $x \in]0,\infty[$ and $n = 1,2,3,\ldots$. Set $Q^n = Q_1^n - Q_2^n - Q_3^n + Q_4^n$ and $Q = Q_1 - Q_2 - Q_3 + Q_4$.

Lemma 4.2.2. *Suppose $(f^n)_{n\in\mathbb{N}} \subset X^+$, $f \in X^+$, where $||f^n|| \leq L$, and $f^n \rightharpoonup f$ in $L^1]0,\infty[$ as $n \to \infty$. Then for each $R > 0$*

$$Q^n(f^n) \rightharpoonup Q(f) \ \text{ in } \ L^1]0,R[\ \text{ as } \ n \to \infty.$$

Proof. Let χ denotes the characteristic function. Choose $R > 0$ and let $\phi \in L^\infty]0, \infty[$. We show that $Q_i^n(f^n) \rightharpoonup Q_i(f)$ in $L^1]0, R[$ as $n \to \infty$ for $i = 1, 2, 3, 4$.

Case $i = 1, 2$
By proceeding the same computation as in Chapter 2, we can easily obtain

$$Q_i^n(f^n) \rightharpoonup Q_i(f) \;\text{ in }\; L^1]0, R[\;\text{ as }\; n \to \infty. \tag{4.18}$$

Case $i = 3$

For a.e. $x \in]0, R]$, by using (H6) we find that

$$|\phi(x)S(x)| \le \|\phi\|_{L^\infty]0,R[}\|S\|_{L^\infty]0,R[}.$$

Then

$$\chi_{]0,R[}\phi S \in L^\infty]0, \infty[. \tag{4.19}$$

Thus by (4.19) and since $f^n \rightharpoonup f$ in $L^1]0, \infty[$ as $n \to \infty$, we obtain

$$\begin{aligned}\Big|\int_0^R &\phi(x)\{Q_3^n(f^n)(x) - Q_3(f)(x)\}dx\Big| \\ &= \Big|\int_0^R \phi(x)S(x)\{f^n(x) - f(x)\}dx\Big| \to 0 \;\text{ as }\; n \to \infty.\end{aligned}$$

Thus by the arbitrariness of ϕ it follows that

$$Q_3^n(f^n) \rightharpoonup Q_3(f) \;\; in \;\; L^1]0, R[\;\text{ as }\; n \to \infty. \tag{4.20}$$

Case $i = 4$

Consider next $\phi \in L^\infty]0, R[$ and compute, for $r > R$,

$$\begin{aligned}\Big|\int_0^R &\phi(x)\{Q_4^n(f^n)(x) - Q_4(f)(x)\}dx\Big| \\ &= \Big|\int_0^R \int_x^\infty \phi(x)S(y)b(x, y)\{f^n(y) - f(y)\}dydx\Big| \\ &= \Big|\int_0^R \int_0^y \phi(x)\Gamma(y, x)\{f^n(y) - f(y)\}dxdy \\ &\quad + \int_R^\infty \int_0^R \phi(x)\Gamma(y, x)\{f^n(y) - f(y)\}dxdy\Big|.\end{aligned}$$

This can be further written as

$$\begin{aligned}
&\left|\int_0^R \phi(x)\{Q_4^n(f^n)(x) - Q_4(f)(x)\}dx\right| \\
&\quad \le \underbrace{\left|\int_0^R \{f^n(y) - f(y)\}\int_0^y \phi(x)\Gamma(y,x)dxdy\right|}_{=:J_1^n} \\
&\quad + \underbrace{\left|\int_R^r \{f^n(y) - f(y)\}\int_0^R \phi(x)\Gamma(y,x)dxdy\right|}_{=:J_2^n} \\
&\quad + \underbrace{\left|\int_r^\infty \{f^n(y) - f(y)\}\int_0^R \phi(x)\Gamma(y,x)dxdy\right|}_{=:J_3^n}. \qquad (4.21)
\end{aligned}$$

We use (H6) and (4.4) to observe that, for $y \in]0, R[$

$$\begin{aligned}
\left|\int_0^y \phi(x)\Gamma(y,x)dx\right| &\le \|S\|_{L^\infty]0,R[}\|\phi\|_{L^\infty]0,R[}\int_0^y b(x,y)dx \\
&\le N\|S\|_{L^\infty]0,R[}\|\phi\|_{L^\infty]0,R[}.
\end{aligned}$$

This shows that the function $y \mapsto \int_0^y \phi(x)\Gamma(y,x)dx$ belongs to $L^\infty]0, R[$. Since $f^n \rightharpoonup f$ in $L^1]0, \infty[$ as $n \to \infty$, it thus follows that

$$\lim_{n\to\infty} J_1^n = 0. \qquad (4.22)$$

Next, in a similar way, one shows that

$$\lim_{n\to\infty} J_2^n = 0. \qquad (4.23)$$

Finally, by using (H4) and Lemma 4.2.1(i) we have

$$\begin{aligned}
&\left|\int_r^\infty \{f^n(y) - f(y)\}\int_0^R \phi(x)\Gamma(y,x)dxdy\right| \\
&\qquad \le k'(R)\|\phi\|_{L^\infty]0,R[}\int_r^\infty y^\theta\{f^n(y) + f(y)\}dy \\
&\qquad \le \frac{2}{r^{1-\theta}}k'(R)\|\phi\|_{L^\infty]0,R[}L
\end{aligned}$$

which is asymptotically small (as $r \to \infty$) uniformly with respect to n. We thus conclude that, also,

$$\lim_{n\to\infty} J_3^n = 0. \qquad (4.24)$$

Thus, by substituting (4.22), (4.23) and (4.24) into (4.21), we obtain

$$\left| \int_0^R \phi(x)\{Q_4^n(f^n)(x) - Q_4(f)(x)\}dx \right| \to 0 \quad \text{as} \quad n \to \infty.$$

Thus by the arbitrariness of ϕ we have

$$Q_4^n(f^n) \rightharpoonup Q_4(f) \quad in \quad L^1]0,R[\quad \text{as} \quad n \to \infty. \tag{4.25}$$

Lemma 4.2.2 follows from (4.18), (4.20) and (4.25).

□

4.2.4 Main result

Now we are in a position to state and prove the main result.

Theorem 4.2.3. *Suppose that (H1), (H2), (H3), (H4), (H5) and (H6) hold and assume that $f_0 \in X^+$. Then (4.1) has a solution f on $]0,\infty[$.*

Proof. Choose $R > 0$, $T > 0$, and let $(f^n)_{n\in\mathbb{N}}$ be the subsequence of approximating solutions obtained above. We have from subsection 4.2.1, for $t \in [0,T]$

$$f^n(t) \rightharpoonup f(t) \quad in \quad L^1]0,R[\quad \text{as} \quad n \to \infty. \tag{4.26}$$

For any $l > 0$, since we know $f^n \rightharpoonup f$ in $L^1]0,\infty[$, we obtain

$$\int_0^l xf(x,t)dx = \lim_{n\to\infty} \int_0^l xf^n(x,t)dx \le \|f_0\|_x < \infty \tag{4.27}$$

using (4.8), the non-negativity of each f^n and f, and then $l \to \infty$ implies that $f \in X^+$. Let $\phi \in L^\infty]0,R[$. From Lemma 4.2.2 we have for each $s \in [0,t]$

$$\int_0^R \phi(x)\{Q^n(f^n(s))(x) - Q(f(s))(x)\}dx \to 0 \quad as \quad n \to \infty. \tag{4.28}$$

Also, for $s \in [0,t]$, using Young's Theorem for convolutions and Lemma 4.2.1 (i)

$$\begin{aligned}
&\int_0^R |\phi(x)||Q^n(f^n(s))(x) - Q(f(s))(x)|dx \\
&\le \|\phi\|_{L^\infty]0,R[}\Big\{\frac{1}{2}\int_0^R\int_0^x K(x-y,y)\{f^n(x-y,s)f^n(y,s) + f(x-y,s)f(y,s)\}dydx \\
&+ \int_0^R\int_0^{n-x} K(x,y)f^n(x,s)f^n(y,s)dydx + \int_0^R\int_0^\infty K(x,y)f(x,s)f(y,s)dydx \\
&+ \int_0^R S(x)\{f^n(x,s) + f(x,s)\}dx \\
&+ \int_0^R\int_x^n S(y)b(x,y)f^n(y,s)dydx + \int_0^R\int_x^\infty S(y)b(x,y)f(y,s)dydx\Big\} \\
&\le \|\phi\|_{L^\infty]0,R[}[3k_1^2L^2 + 2\{\omega(R,R) + Rk(R) + \|S\|_{L^\infty]0,R[}\}L].
\end{aligned} \tag{4.29}$$

Since the left-hand side of (4.29) is in $L^1]0,t[$ we have by (4.28), (4.29) and the dominated convergence theorem

$$\left|\int_0^t \int_0^R \phi(x)\{Q^n(f^n(s))(x) - Q(f(s))(x)\}dxds\right| \to 0 \quad \text{as} \quad n \to \infty. \tag{4.30}$$

Since ϕ is arbitrary, and the equation (4.30) holds for all $\phi \in L^\infty]0,R[$, by the application of Fubini's Theorem we obtain

$$\int_0^t Q^n(f^n(s))ds \rightharpoonup \int_0^t Q(f(s))ds \quad \text{in} \quad L^1]0,R[\quad \text{as} \quad n \to \infty. \tag{4.31}$$

From the definition of Q^n and equation (4.6) we have for $t \in [0,T]$

$$f^n(x,t) = \int_0^t Q^n(f^n(s))(x)ds + f^n(x,0),$$

and thus it follows from (4.31)and (4.26) that

$$\int_0^R \phi(x)f(x,t)dx = \int_0^t \int_0^R \phi(x)Q(f(s))(x)dxds + \int_0^R \phi(x)f(x,0)dx,$$

for any $\phi \in L^\infty]0,R]$. Therefore it holds for all $\phi \in C_0^\infty(]0,R])$. This implies for almost any x in $]0,R]$ we have

$$f(x,t) = \int_0^t Q(f(s))(x)ds + f(x,0).$$

It now follows from the arbitrariness of T and R that f is a solution to (4.1) on $[0,\infty[$. This completes the proof of Theorem 4.2.3. □

Chapter 5

Convergence analysis of the fixed pivot technique for coagulation equation

This chapter contains a detailed study of convergence analysis for the fixed pivot technique given by S. Kumar and Ramkrishna [54] for the nonlinear pure coagulation equations. In particular, we investigate the convergence for five different types of uniform and non-uniform meshes which turns out that the fixed pivot technique is second order convergent on a uniform and non-uniform smooth meshes. Moreover, it yields first order convergence on a locally uniform mesh. Finally the analysis exhibits that the method does not converge on oscillatory and non-uniform random meshes. The mathematical results of the convergence analysis are also demonstrated numerically.

Let us now briefly outline the contents of this chapter. The following section provides a short introduction of the problem. Along with the general idea of sectional methods, a concise review of the mathematical formulation of the fixed pivot technique is given in Section 5.2. Some useful definitions and a theorem from Hundsdorfer and Verwer [44] used in further analysis as well as the main result for the convergence of the fixed pivot technique are also stated in Section 5.2. To show the convergence of the scheme, the consistency and Lipschitz conditions are discussed in Sections 5.3 and 5.4, respectively. Numerical simulations are performed in Section 5.5.

5.1 Introduction

The nonlinear continuous coagulation equation is given by, see [71]

$$\frac{\partial f(t,x)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)f(t,x-y)f(t,y)dy - \int_0^\infty K(x,y)f(t,x)f(t,y)dy, \quad (5.1)$$

with

$$f(x,0) = f^{\text{in}}(x) \geq 0, \quad x \in]0,\infty[.$$

where the variables $x > 0$ and $t \geq 0$ denote the size of the particles and time respectively. The number density of particles of size x at time t is denoted by $f(x,t) \geq 0$. The coagulation kernel $K(x,y) \geq 0$ represents the rate at which particles of size x coalesce with those of size y. It will be assumed throughout that $K(x,y) = K(y,x)$ for all x, $y > 0$, i.e. symmetric.

Mathematical results on existence and uniqueness of solutions to equation (5.1) can be found in [18, 21, 27, 56, 57, 65, 66, 60, 89] for different classes of coagulation kernels. However, for the sake of simplicity in our analysis we consider them to be twice continuously differentiable functions. The pure coagulation equation (5.1) can be solved analytically only for some limited class of coagulation kernels, see [20, 33, 34]. Due to limited availability of analytical solutions, it is of great interest to develop new numerical techniques to solve these equations and assess them by means of mathematical analysis. In the pure coagulation equation (5.1) the volume variable x ranges from 0 to ∞. In order to apply a numerical scheme to the solution of the equation, the initial step is to set a finite computational domain. In this work we consider the following truncated equation

$$\frac{\partial n(t,x)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)n(t,x-y)n(t,y)dy - \int_0^{x_{\max}} K(x,y)n(t,x)n(t,y)dy, \quad (5.2)$$

with

$$n(x,0) = n^{\text{in}}(x) \geq 0, \quad x \in \Omega :=]0, x_{\max}].$$

Here the variable $n(t,x)$ represents the solution to the preceding truncated equation. The existence and uniqueness of non-negative solutions for the truncated pure coagulation equation (5.2) has been derived in [4, 15, 21, 89]. In [21, 27, 89], it is proven that the sequence of solutions to the truncated problems converge weakly to the solution of the original problem in a weighted L^1 space as $x_{\max} \to \infty$ for certain classes of kernels.

5.2 The sectional methods

Sectional methods can be described by the following general mathematical derivation. These methods approximate the total number of particles in finite number of cells.

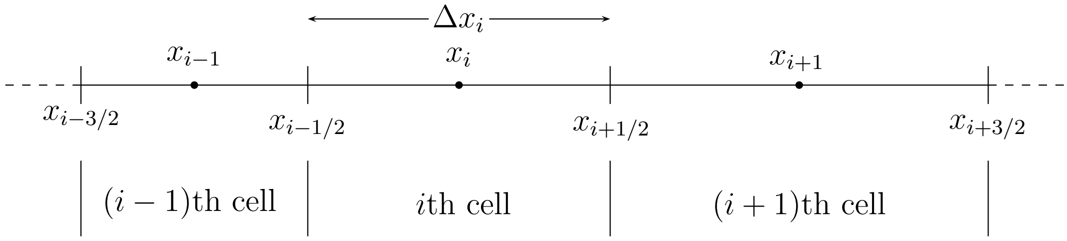


Figure 5.1: A discretized size domain.

As a first step, the continuous interval $\Omega :=]0, x_{\max}]$ is divided into a small number of cells defining size classes

$$\Lambda_i :=]x_{i-1/2}, x_{i+1/2}],\ i = 1, \ldots, I,$$

with

$$x_{1/2} = 0, \quad x_{I+1/2} = x_{\max}, \quad \Delta x_{\min} \leq \Delta x_i = x_{i+1/2} - x_{i-1/2} \leq \Delta x.$$

For the purpose of later analysis we assume quasi uniformity of the grids, i.e.

$$\frac{\Delta x}{\Delta x_{\min}} \leq C \tag{5.3}$$

where C is a positive constant. The representative of each size class, usually the center point of each cell $x_i = (x_{i-1/2} + x_{i+1/2})/2$, is called pivot or grid point. This type of partitioning of the spatial domain is known as *cell centered* representation of the mesh. A typical cell centered partitioning of the domain is shown in Figure 5.1. The integration of the equation (5.2) over each cell yields a *semi-discrete* system in $\mathbb{R}^I$

$$\frac{d\mathbf{N}}{dt} = \mathbf{B} - \mathbf{D}, \tag{5.4}$$

$$\mathbf{N}(0) = \mathbf{N}^{\text{in}}.$$

Here we consider $\mathbf{N}^{\text{in}}, \mathbf{N}, \mathbf{B}, \mathbf{D} \in \mathbb{R}^I$ whose semi-discrete ith components are defined as

$$N_i(t) = \int_{x_{i-1/2}}^{x_{i+1/2}} n(t, x)dx, \tag{5.5}$$

$$N_i^{\text{in}} = \int_{x_{i-1/2}}^{x_{i+1/2}} n^{\text{in}}(x)dx,$$

$$B_i = \frac{1}{2} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x K(x - y, y)n(t, x - y)n(t, y)dydx. \tag{5.6}$$

and

$$D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} K(x,y)n(t,y)n(t,x)dydx. \tag{5.7}$$

Here the vector $\mathbf{N}$ is formed by the vector of values of the step function obtained by L^2 projection of the exact solution n into the space of step functions constant on each cell. Note that this projection error can easily be shown of second order, see Subsection 5.2.2. Various sectional methods for the numerical solutions of the equation (5.2) can be obtained from different choices of numerical approximations of B_i and D_i in terms of $N_i(t)$. Finally the sectional methods take the following spatially discretized form

$$\frac{d\hat{\mathbf{N}}}{dt} = \hat{\mathbf{B}}(\hat{\mathbf{N}}) - \hat{\mathbf{D}}(\hat{\mathbf{N}}) =: \hat{\mathbf{F}}(t, \hat{\mathbf{N}}), \tag{5.8}$$

$$\hat{\mathbf{N}}(0) = \mathbf{N}^{\text{in}}, \tag{5.9}$$

where $\hat{\mathbf{B}}, \hat{\mathbf{D}} \in \mathbb{R}^I$ are some functions of $\hat{\mathbf{N}}$. The ith component, $\hat{N}_i(t)$ of the vector $\hat{\mathbf{N}}$ is the numerical approximation of the total number in ith cell $N_i(t)$.

5.2.1 The fixed pivot technique

The fixed pivot technique is based on the idea of birth modification. According to Kumar and Ramkrishna [54], the equation (5.2) is modified to

$$\begin{aligned}\frac{d}{dt}\int_{x_{i-1/2}}^{x_{i+1/2}} n(t,x)dx \approx & \frac{1}{2}\int_{x_i}^{x_{i+1}} \lambda_i^+(x) \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx \\ &+ \frac{1}{2}\int_{x_{i-1}}^{x_i} \lambda_i^-(x) \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx \\ &- \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} K(x,y)n(t,y)n(t,x)dydx. \end{aligned} \tag{5.10}$$

where

$$\lambda_i^{\pm}(x) = \frac{x - x_{i\pm1}}{x_i - x_{i\pm1}}. \tag{5.11}$$

Now substituting the number density approximation

$$n(t,x) \approx \sum_{i=1}^{I} N_i(t)\delta(x - x_i),$$

into the preceding equation, we obtain the following spatially discretized system

$$
\begin{aligned}
\frac{dN_i(t)}{dt} = & \sum_{x_i \le x_j + x_k < x_{i+1}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) \lambda_i^+ (x_k + x_j) K(x_k, x_j) N_j N_k \\
& + \sum_{x_{i-1} \le x_j + x_k < x_i}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) \lambda_i^- (x_k + x_j) K(x_k, x_j) N_j N_k \\
& - N_i \sum_{j=1}^{I} K(x_i, x_j) N_j, \quad i = 1, \ldots, I \\
= & \hat{B}_i^{FP} - \hat{D}_i^{FP}, \quad i = 1, \ldots, I
\end{aligned} \tag{5.12}
$$

where $\hat{B}_i^{FP}$ and $\hat{D}_i^{FP}$ represent the birth and death terms, respectively in the ith cell obtained from the fixed pivot technique. The basic idea of the fixed pivot technique can be described as follows. Assume that a new born particle of a size, which is not positioned at a pivot point of any cell, appears due to the aggregation of two smaller particles. The particle has to be assigned onto neighboring pivot points in such a way that the particles number and mass are conserved. This problem can be solved in a unique way. The resulting technique very often gives quite satisfactory results. However, the undesirable part is that the fixed pivot technique turns into a zero order method on oscillatory and non-uniform random meshes for aggregation problems. At the last boundary cell Kumar and Ramkrishna simply set the first integral on the right hand side in (5.10) to be zero in their numerical computations. However, we have observed in our analysis for the aggregation problem that this setting at the end boundary reduces by one order the accuracy of the fixed pivot technique. To overcome this problem, we take an extra grid point x_{I+1} at a Δx_I distance away from the grid point x_I. In the computations contributions that are larger than x_I are distributed to x_I and x_{I+1}. This is used in Lemma 5.3.1. A similar modification should also be used at the first boundary cell for breakage problems in J. Kumar and Warnecke [51].

It should be mentioned here that in this work we consider the following L_1 norm

$$\|\mathbf{N}\| = \sum_{i=1}^{I} |N_i|.$$

We consider $\mathcal{C}^2([a, b])$ as a space of two times continuously differentiable functions on $]a, b[$ with finite limits of the functions and their first as well as second derivatives at a and b. Note that for the sake of simplicity in our analysis we assume that the aggregation kernel and number density

$$K \in \mathcal{C}^2([0, x_{\max}] \times [0, x_{\max}]) \quad \text{and} \quad n \in \mathcal{C}^2([0, x_{max}]) \tag{5.13}$$

respectively.

5.2.2 Projection error and spatially discretization error

Let $\hat{n}(t)$ for some $t \in [0, \infty[$ be the numerical solution of the problem (5.2) which has a weak solution n in the L_1^1 space. The norm on L_1^1 is the same as is on X^+ in Chapters 2 and 3. Then the convergence error is defined as

$$e_c(t, \cdot) = n(t, \cdot) - I_{\Delta x}\hat{n}(t). \tag{5.14}$$

where

$$I_{\Delta x}\hat{n}(t) := \sum_{i=1}^{I} \hat{n}_i(t)\varphi_i,$$

with

$$\varphi_i(x) := \begin{cases} 1 & \text{if } x \in \Lambda_i, \\ 0 & \text{elsewhere.} \end{cases}$$

Suppose $\tilde{n}$ is a vector in $\mathbb{R}^I$ whose ith component is defined as follows

$$\tilde{n}_i(t) = \frac{N_i(t)}{\Delta x_i} = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} n(t, x)dx.$$

Using

$$I_{\Delta x}n(t, \cdot) = \sum_{i=1}^{I} \tilde{n}_i(t)\varphi_i,$$

we define the projection of elements in L_1^1 onto step functions with respect to the mesh. Taking the norm on both sides in (5.14), we estimate

$$\|e_c(t, \cdot)\| \leq \|n(t, \cdot) - I_{\Delta x}n(t, \cdot)\|_{L_1^1} + \|I_{\Delta x}n(t, \cdot) - I_{\Delta x}\hat{n}(t)\|_{L_1^1}. \tag{5.15}$$

The first and second terms on the right hand side in (5.15) represent the *projection error* and *spatially discretization error*, respectively for the number density n. Let us now calculate each error separately.

First, we consider the projection error from (5.15) as

$$\begin{aligned}
\|n(t,\cdot)-I_{\Delta x}n(t,\cdot)\|_{L^1_1} =& \int_0^{x_{\max}} (1+x)|n(t,x)-I_{\Delta x}n(t,x)|dx \\
=& \sum_{i=1}^{I}\int_{\Lambda_i}(1+x)|n(t,x)-I_{\Delta x}n(t,x)|dx \\
\leq& (1+x_{\max})\sum_{i=1}^{I}\int_{\Lambda_i}|n(t,x)-\tilde{n}_i|dx \\
=& (1+x_{\max})\sum_{i=1}^{I}\left[\int_{\Lambda_i}|n(t,x)-\tilde{n}_i|dx-|n(t,x_i)-\tilde{n}_i|\Delta x_i\right] \\
&+(1+x_{\max})\sum_{i=1}^{I}|n(t,x_i)-\tilde{n}_i|\Delta x_i.
\end{aligned}$$

Applying the midpoint rule twice, once in the integral that appears in the first term and then in the definition of $\tilde{n}_i$ for the second term on the right hand side, one can obtain

$$\|n(t,\cdot)-I_{\Delta x}n(t,\cdot)\|_{L^1_1} \leq (1+x_{\max})\mathcal{O}(\Delta x^2).$$

Next, we take the spatially discretization error from (5.15) as

$$\begin{aligned}
\|I_{\Delta x}n(t,\cdot)-I_{\Delta x}\hat{n}(t)\|_{L^1_1} =& \left\|\sum_{i=1}^{I}(\tilde{n}_i-\hat{n}_i)\varphi_i(x)\right\|_{L^1_1} \\
\leq& \int_0^{x_{\max}}(1+x)\sum_{i=1}^{I}|\tilde{n}_i-\hat{n}_i||\varphi_i(x)|dx \\
\leq& (1+x_{\max})\sum_{i=1}^{I}|\tilde{n}_i-\hat{n}_i|\int_{\Lambda_i}|\varphi_i(x)|dx \\
\leq& (1+x_{\max})\sum_{i=1}^{I}\left|\frac{N_i}{\Delta x_i}-\frac{\hat{N}_i}{\Delta x_i}\right|\Delta x_i \\
\leq& (1+x_{\max})\sum_{i=1}^{I}|N_i-\hat{N}_i| \\
=& (1+x_{\max})\|\mathbf{N}-\hat{\mathbf{N}}\|.
\end{aligned}$$

Finally we substitute the estimates on the projection error and spatially discretized error in (5.15) to obtain

$$\|e_c(t,\cdot)\| \leq (1+x_{\max})[\|\mathbf{N}-\hat{\mathbf{N}}\|+\mathcal{O}(\Delta x^2)].$$

So the order of convergence may depend on $\|\mathbf{N}-\hat{\mathbf{N}}\|$. Therefore, the purpose of rest of the chapter is to check the convergence of the scheme (5.8).

As we move on to the subsequent sections, it will be helpful to revisit some definitions and an existing theorem given in Hundsdorfer and Verwer [44]. These will be of use while discussing in detail the consistency and the convergence of the fixed pivot technique.

Definition 5.2.1. *The **spatial truncation error** is defined by the residual left by substituting the exact solution* $\mathbf{N}(t)$ *into equation (5.8) as*

$$\sigma(t) = \frac{d\mathbf{N}(t)}{dt} - \left(\hat{\mathbf{B}}\left(\mathbf{N}(t)\right) - \hat{\mathbf{D}}\left(\mathbf{N}(t)\right)\right). \tag{5.16}$$

The scheme (5.8) is called consistent of order p *if, for* $\Delta x \to 0$,

$$\|\sigma(t)\| = \mathcal{O}(\Delta x^p), \quad \text{uniformly for all } t,\ 0 \le t \le T.$$

Definition 5.2.2. *The **global discretization error** is defined by*

$$\epsilon(t) = \mathbf{N}(t) - \hat{\mathbf{N}}(t). \tag{5.17}$$

The scheme (5.8) is called convergent of order p *if, for* $\Delta x \to 0$,

$$\|\epsilon(t)\| = \mathcal{O}(\Delta x^p), \quad \text{uniformly for all } t,\ 0 \le t \le T.$$

It is important that the solution obtained by the fixed pivot technique remains non-negative for all times. This is shown in proposition 5.4.1 by using the next well known theorem. In the following theorem we consider $\hat{\mathbf{M}} \ge 0$ for a vector $\hat{\mathbf{M}} \in \mathbb{R}^I$ if all of its components are non-negative.

Theorem 5.2.3. *(Hundsdorfer and Verwer [44]). Suppose that* $\hat{\mathbf{F}}(t, \hat{\mathbf{M}})$ *is continuous and satisfies the Lipschitz condition*

$$\|\hat{\mathbf{F}}(t, \hat{\mathbf{P}}) - \hat{\mathbf{F}}(t, \hat{\mathbf{M}})\| \le L\|\hat{\mathbf{P}} - \hat{\mathbf{M}}\| \quad \text{for all } \ \hat{\mathbf{P}}, \hat{\mathbf{M}} \in \mathbb{R}^I.$$

Then the solution of the semi-discrete system (5.8) is non-negative if and only if for any vector $\hat{\mathbf{M}} \in \mathbb{R}^I$ *with* $\hat{\mathbf{M}} \ge 0$ *we have for any* $i = 1, \dots, I$ *and all* $t \ge 0$ *that* $\hat{M}_i = 0$ *implies* $\hat{F}_i(t, \hat{\mathbf{M}}) \ge 0$.

Proof. The proof can be found in Hundsdorfer and Verwer [44], Chap. 1, Theorem 7.1. □

Now we shall state the main result which helps us to show the convergence of the fixed pivot technique.

Theorem 5.2.4. *Let us assume that the Lipschitz conditions on* $\hat{\mathbf{B}}(\mathbf{N}(t))$ *and* $\hat{\mathbf{D}}(\mathbf{N}(t))$ *are satisfied for* $0 \le t \le T$ *and for all* $\mathbf{N}$, $\hat{\mathbf{N}} \in \mathbb{R}^I$ *where* $\mathbf{N}$ *and* $\hat{\mathbf{N}}$ *are the projected exact and numerical solutions defined in (5.4) and (5.8) respectively. Then a consistent discretization method is also convergent and the convergence is of the same order as the consistency.*

To fulfill the requirements of Theorem 5.2.4, for the convergence of the fixed pivot technique we need to prove that the scheme is consistent and the birth $\hat{\mathbf{B}}(\mathbf{N}(t))$ and death $\hat{\mathbf{D}}(\mathbf{N}(t))$ terms satisfy the Lipschitz conditions.

5.3 Consistency

We need the following lemma from [51] to investigate the consistency of the fixed pivot technique. For the completeness, we will also repeat the proof.

Lemma 5.3.1. *Consider a function $f \in \mathcal{C}^2([0, x_{max}])$ and a cell centered partitioning of the domain $[0, x_{max}]$ given as $0 = x_{1-1/2} < \ldots < x_{i-1/2} < x_{i+1/2} < \ldots < x_{I+1/2} = x_{max}$ with pivot points $x_i = (x_{i-1/2} + x_{i+1/2})/2$ and a bound $\Delta x \geq \Delta x_i = (x_{i+1/2} - x_{i-1/2})$ for all i. If $\lambda_i^+(x)$ and $\lambda_i^-(x)$ are given by the relation (5.11), then the following approximations can be obtained*

$$\begin{aligned}\int_{x_{i-1/2}}^{x_{i+1/2}} f(x)dx = &\int_{x_i}^{x_{i+1}} \lambda_i^+(x)f(x)dx + \int_{x_{i-1}}^{x_i} \lambda_i^-(x)f(x)dx \\ &+ \frac{f(x_i)}{2}\left[\Delta x_i - \left(\frac{\Delta x_{i-1} + \Delta x_{i+1}}{2}\right)\right] \\ &- \frac{f'(x_i)}{12}\left[(\Delta x_{i+1} - \Delta x_{i-1})\left\{\Delta x_i + \left(\frac{\Delta x_{i-1} + \Delta x_{i+1}}{2}\right)\right\}\right] \\ &+ \mathcal{O}(\Delta x^3), \quad \textit{for} \;\; i = 2, \ldots, I-1,\end{aligned}$$

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f(x)dx = \int_{x_i}^{x_{i+1}} \lambda_i^+(x)f(x)dx + \int_{x_{i-1}}^{x_i} \lambda_i^-(x)f(x)dx + \frac{f(x_i)}{4}[\Delta x_i - \Delta x_{i-1}] + \mathcal{O}(\Delta x^2), \quad \textit{for} \;\; i = I,$$

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f(x)dx = \int_{x_i}^{x_{i+1}} \lambda_i^+(x)f(x)dx + \frac{f(x_i)}{4}[3\Delta x_i - \Delta x_{i+1}] + \mathcal{O}(\Delta x^2), \quad \textit{for} \;\; i = 1.$$

Note that x_{I+1} is the extra grid point introduced in subsection 5.2.1.

Proof. First, we consider the cases $i = 2, \ldots I-1$ and denote the following expression by $\mathfrak{I}_i$.

$$\mathfrak{I}_i(f) = \int_{x_{i-1/2}}^{x_{i+1/2}} f(x)\,dx - \left(\int_{x_i}^{x_{i+1}} \lambda_i^+(x)f(x)\,dx + \int_{x_{i-1}}^{x_i} \lambda_i^-(x)f(x)\,dx\right).$$

Taylor series expansion of $f(x)$ about x_i in $\mathfrak{I}_i$ yields

$$\begin{aligned}\mathfrak{I}_i(f) =&f(x_i)\left[\Delta x_i - \left(\int_{x_i}^{x_{i+1}} \lambda_i^+(x)dx + \int_{x_{i-1}}^{x_i} \lambda_i^-(x)dx\right)\right] \\ &- f'(x_i)\left(\int_{x_i}^{x_{i+1}} \lambda_i^+(x)(x - x_i)dx + \int_{x_{i-1}}^{x_i} \lambda_i^-(x)(x - x_i)dx\right) + \mathcal{O}(\Delta x^3).\end{aligned}$$

Substituting the values of λ_i^+ and λ_i^- from (5.11) into the preceding equation, we obtain

$$\begin{aligned}\mathfrak{I}_i(f) =& f(x_i)\left[\Delta x_i - \frac{1}{2}(x_{i+1}-x_{i-1})\right] \\ &- \frac{f'(x_i)}{6}\Big[(x_{i+1}-x_{i-1})\big\{(x_{i+1}-x_i)-(x_i-x_{i-1})\big\}\Big] + \mathcal{O}(\Delta x^3). \qquad (5.18)\end{aligned}$$

For the cell centered grids, i.e. $x_i = (x_{i-1/2}+x_{i+1/2})/2$, the equation (5.18) becomes

$$\begin{aligned}\mathfrak{I}_i(f) =& \frac{f(x_i)}{2}\left[\Delta x_i - \frac{1}{2}(\Delta x_{i+1}+\Delta x_{i-1})\right] \\ &- \frac{f'(x_i)}{12}\left[(\Delta x_{i+1}-\Delta x_{i-1})\left\{\Delta x_i + \left(\frac{\Delta x_{i-1}+\Delta x_{i+1}}{2}\right)\right\}\right] + \mathcal{O}(\Delta x^3).\end{aligned}$$

Next, we take $i = I$

$$\mathfrak{I}_I(f) = \int_{x_{I-1/2}}^{x_{I+1/2}} f(x)dx - \int_{x_I}^{x_{I+1}} \lambda_I^+(x)f(x)dx - \int_{x_{I-1}}^{x_I} \lambda_I^-(x)f(x)dx.$$

Applying the midpoint, left rectangle and right rectangle rules in first, second and thirds integrals respectively, we get

$$\begin{aligned}\mathfrak{I}_I(f) =& f(x_I)\Delta x_I - \left[\lambda_I^+(x_I)f(x_I)(x_{I+1}-x_I) - \frac{f(x_I)}{2}(x_{I+1}-x_I)\right] \\ &- \left[\lambda_I^-(x_I)f(x_I)(x_I-x_{I-1}) - \frac{f(x_I)}{2}(x_I-x_{I-1})\right] + \mathcal{O}(\Delta x^2) \\ =& f(x_I)\Delta x_I - \frac{f(x_I)}{2}(x_{I+1}-x_I) - \frac{f(x_I)}{2}(x_I-x_{I-1}) + \mathcal{O}(\Delta x^2) \\ =& f(x_I)\left[\Delta x_I - \frac{1}{2}\Delta x_I - \frac{1}{4}(\Delta x_I + \Delta x_{I-1})\right] + \mathcal{O}(\Delta x^2) \\ =& \frac{f(x_I)}{4}(\Delta x_I - \Delta x_{I-1}) + \mathcal{O}(\Delta x^2).\end{aligned}$$

Now we consider $i = 1$

$$\mathfrak{I}_1(f) = \int_{x_{1/2}}^{x_{3/2}} f(x)dx - \int_{x_1}^{x_2} \lambda_I^+(x)f(x)dx.$$

We apply midpoint and left rectangle rules in first and second integrals respectively to obtain

$$\begin{aligned}\mathfrak{I}_1(f) =& f(x_1)\Delta x_1 - \left[\lambda_1^+(x_1)f(x_1)(x_2-x_1) - \frac{f(x_1)}{2}(x_2-x_1)\right] + \mathcal{O}(\Delta x^2) \\ =& f(x_1)\left[\Delta x_1 - \frac{1}{4}(\Delta x_1+\Delta x_2)\right] \\ =& \frac{f(x_1)}{4}(3\Delta x_1 - \Delta x_2).\end{aligned}$$

Hence the proof of Lemma 5.3.1 is completed. □

Now we describe the three main subsections to inquire the consistency of the fixed pivot technique. We evaluate the order of the birth term and the order of the death term with the brief summary of all terms in Subsections 5.3.1 and 5.3.2, respectively. Finally, we consider five different types of meshes to evaluate the local discretization error in Subsection 5.3.3.

5.3.1 Order of the birth term

The integrated birth term can be written as follows

$$B_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx.$$

Let us denote

$$f(t,x) = \frac{1}{2}\int_0^x K(x-y,y)n(t,x-y)n(t,y)dy. \tag{5.19}$$

Birth term on internal cells

Considering $i = 2,\dots,I-1$ and using Lemma 5.3.1, we can rewrite B_i as

$$\begin{aligned}B_i =& \frac{1}{2}\int_{x_i}^{x_{i+1}} \lambda_i^+(x)\int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx \\ &+ \frac{1}{2}\int_{x_{i-1}}^{x_i} \lambda_i^-(x)\int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx + \mathfrak{J}_i(f).\end{aligned}$$

By changing the order of integration of the first two terms on the right hand side, we obtain

$$\begin{aligned}B_i =& \frac{1}{2}\int_0^{x_i}\int_{x_i}^{x_{i+1}} \lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\ &+ \frac{1}{2}\int_{x_i}^{x_{i+1}}\int_y^{x_{i+1}} \lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\ &+ \frac{1}{2}\int_0^{x_{i-1}}\int_{x_{i-1}}^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\ &+ \frac{1}{2}\int_{x_{i-1}}^{x_i}\int_y^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy + \mathfrak{J}_i(f).\end{aligned}$$

Each integral term on the right hand side can be further rewritten as

$$\begin{aligned}
B_i =& \frac{1}{2}\sum_{j=1}^{i-1}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{x_i}^{x_{i+1}} \lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\
&+\frac{1}{2}\int_{x_{i-1/2}}^{x_i}\int_{x_i}^{x_{i+1}} \lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\
&+\frac{1}{2}\int_{x_i}^{x_{i+1}}\int_{y}^{x_{i+1}} \lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\
&+\frac{1}{2}\sum_{j=1}^{i-2}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{x_{i-1}}^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\
&+\frac{1}{2}\int_{x_{i-3/2}}^{x_{i-1}}\int_{x_{i-1}}^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\
&+\frac{1}{2}\int_{x_{i-1}}^{x_i}\int_{y}^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy+\mathfrak{J}_i(f).
\end{aligned} \tag{5.20}$$

Let us denote the integral terms on the right hand side by $I_1, \ldots, I_6$ respectively and calculate them separately.

The integrals I_6 and I_3.

$$\begin{aligned}
I_6 &= \frac{1}{2}\int_{x_{i-1}}^{x_i}\int_{y}^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\
&= \frac{1}{2}\int_{x_{i-1}}^{x_i} g(t,y)dy,
\end{aligned}$$

where

$$g(t,y) := \int_{y}^{x_i} \lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dx. \tag{5.21}$$

Using Taylor series expansion of $g(t,y)$ with respect to y about x_{i-1}, we get

$$I_6 = g(t,x_{i-1})\frac{(\Delta x_{i-1}+\Delta x_i)}{4} + g_y(t,x_{i-1})\frac{(\Delta x_{i-1}+\Delta x_i)^2}{16} + \ldots, \tag{5.22}$$

where

$$g_y(t,x_{i-1}) = \frac{\partial g}{\partial y}(t,x_{i-1}) = \frac{\partial g}{\partial y}(t,y)|_{y=x_{i-1}}.$$

Now we calculate $g_y(t,x_{i-1})$ using the Leibniz rule to differentiate under an integral using $\lambda_i^-(x_{i-1})=0$

$$\begin{aligned}
g_y(t,x_{i-1}) = &\Bigg[n_y(t,y)\int_y^{x_i}\lambda_i^-(x)K(x-y,y)n(t,x-y)dx\\
&+n(t,y)\frac{\partial}{\partial y}\int_y^{x_i}\lambda_i^-(x)K(x-y,y)n(t,x-y)dx\Bigg]_{y=x_{i-1}},\\
=& n_y(t,x_{i-1})\int_{x_{i-1}}^{x_i}\lambda_i^-(x)K(x-x_{i-1},x_{i-1})n(t,x-x_{i-1})dx\\
&+n(t,x_{i-1})\Bigg[\int_y^{x_i}\lambda_i^-(x)\frac{\partial}{\partial y}\{K(x-y,y)n(t,x-y)\}dx\Bigg]_{y=x_{i-1}},\\
=& n_y(t,x_{i-1})\int_{x_{i-1}}^{x_i}\lambda_i^-(x)K(x-x_{i-1},x_{i-1})n(t,x-x_{i-1})dx\\
&+n(t,x_{i-1})\int_{x_{i-1}}^{x_i}\lambda_i^-(x)\Bigg[\{\frac{\partial}{\partial y}K(x-y,y)\}_{y=x_{i-1}}n(t,x-x_{i-1})\\
&\qquad+K(x-x_{i-1},x_{i-1})n_y(t,x-x_{i-1})\Bigg]dx.
\end{aligned}$$

Then, we apply the left rectangle rule and use $\lambda_i^-(x_{i-1})=0$ and $K(0,x_{i-1})=0$ to get

$$g_y(t,x_{i-1})=0+0+\mathcal{O}(\Delta x^2).$$

Now we have to evaluate $g(t,x_{i-1})$ from the equation (5.21)

$$g(t,x_{i-1})=\int_{x_{i-1}}^{x_i}\lambda_i^-(x)K(x-x_{i-1},x_{i-1})n(t,x-x_{i-1})n(t,x_{i-1})dx.$$

Again apply the left rectangle rule use $\lambda_i^-(x_{i-1})=0$ and $K(0,x_{i-1})=0$, and we obtain

$$g(t,x_{i-1})=0+\mathcal{O}(\Delta x^2).$$

By substituting the value of $g_y(t,x_{i-1})$ and $g(t,x_{i-1})$ in the equation (5.22) we get

$$I_6=0+\mathcal{O}(\Delta x^3). \tag{5.23}$$

Similarly, we can evaluate the third term

$$I_3=0+\mathcal{O}(\Delta x^3). \tag{5.24}$$

The integrals I_1 and I_4.

Now we consider the first term in (5.20)

$$I_1=\frac{1}{2}\sum_{j=1}^{i-1}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{x_i}^{x_{i+1}}\lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy$$

and apply the midpoint rule to get

$$I_1 = \frac{1}{2}\sum_{j=1}^{i-1}\int_{x_i}^{x_{i+1}} \lambda_i^+(x)K(x-x_j,x_j)n(t,x-x_j)dx \times n(t,x_j)\Delta x_j + \mathcal{O}(\Delta x^3).$$

Furthermore we can use the relationship $N_i(t) = n(t,x_i)\Delta x_i + \mathcal{O}(\Delta x^3)$ for the midpoint rule to get the form

$$I_1 = \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i}^{x_{i+1}} \lambda_i^+(x)K(x-x_j,x_j)n(t,x-x_j)dx + \mathcal{O}(\Delta x^3).$$

By using the substitution $x - x_j = x'$ we obtain

$$I_1 = \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i-x_j}^{x_{i+1}-x_j} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' + \mathcal{O}(\Delta x^3). \tag{5.25}$$

We define $l_{i,j}$ and $\gamma_{i,j}$ to be those indices such that the following hold

$$x_i - x_j \in \Lambda_{l_{i,j}} \quad \text{and} \quad \gamma_{i,j} := H[(x_i - x_j) - x_{l_{i,j}}] \tag{5.26}$$

where

$$H(x) := \begin{cases} 1 & \text{if } x > 0, \\ \text{-1} & \text{if } x \leq 0. \end{cases}$$

We will use the convention of Riemann integration that $\int_a^b f(x)dx = -\int_b^a f(x)dx$ and the equation (5.25) can be rewritten as

$$\begin{aligned} I_1 =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \int_{x_{k-1/2}}^{x_{k+1/2}} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1}-x_j} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' + \mathcal{O}(\Delta x^3). \end{aligned}$$

Let $p := \#\left\{n : l_{i,j} + \frac{1}{2}(\gamma_{i,j}+1) \leq n \leq l_{i+1,j} + \frac{1}{2}(\gamma_{i+1,j}-1)\right\}$ to be the total number of terms in the following sum

$$\sum_{k=l_{i,j}+\frac{1}{2}(\gamma_{i,j}+1)}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \int_{x_{k-1/2}}^{x_{k+1/2}} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx'$$

and set

$$k_1 := l_{i,j} + \frac{1}{2}(\gamma_{i,j}+1), \quad k_2 := k_1 + 1, \ldots, \quad k_{p-1} := k_1 + (p-2).$$

Next, we shall show that p is finite. By using the definition of the indices $l_{i,j}$ and $\gamma_{i,j}$ in (5.26), we can estimate

$$(p-2)\Delta x_{\min} \le \Delta x_{k_2} + \Delta x_{k_3} + \ldots + \Delta x_{k_{p-1}} \le \frac{1}{2}(\Delta x_i + \Delta x_{i+1}) \le \Delta x$$

which implies using the assumption of quasi uniformity (5.3) that

$$(p-2) \le \frac{\Delta x}{\Delta x_{\min}} \le C \Rightarrow p \le C+2.$$

This means the above sum has uniformly bounded finite number of terms. So one can apply the midpoint rule in the second term on the right hand side to get

$$\begin{aligned}
I_1 =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \lambda_i^+(x_k+x_j)K(x_k,x_j)n(t,x_k)\Delta x_k \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1}-x_j} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\
&- \frac{1}{12}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} \frac{\partial}{\partial x'}\{K(x_k,x_j)n(t,x_k)\} + \mathcal{O}(\Delta x^3).
\end{aligned}$$

This can be further rewritten as

$$\begin{aligned}
I_1 =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \sum_{x_i\le x_j+x_k<x_{i+1}} \lambda_i^+(x_k+x_j)K(x_k,x_j)N_k \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1}-x_j} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\
&- \frac{1}{12}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} \frac{\partial}{\partial x'}\{K(x_k,x_j)n(t,x_k)\} + \mathcal{O}(\Delta x^3). \quad (5.27)
\end{aligned}$$

Now we consider the fourth term given by

$$I_4 = \frac{1}{2}\sum_{j=1}^{i-2}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{x_{i-1}}^{x_i}\lambda_i^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy.$$

Similarly as before, we obtain

$$\begin{aligned}
I_4 =& \frac{1}{2}\sum_{j=1}^{i-2}N_j\int_{x_{i-1}-x_j}^{x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}}\lambda_i^-(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-2}N_j\sum_{k=l_{i-1,j}+\frac{1}{2}(1+\gamma_{i-1,j})}^{l_{i,j}+\frac{1}{2}(\gamma_{i,j}-1)}\lambda_i^-(x_k+x_j)K(x_k,x_j)n(t,x_k)\Delta x_k \\
&+ \frac{1}{2}\sum_{j=1}^{i-2}N_j\int_{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}}^{x_i-x_j}\lambda_i^-(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{12}\sum_{j=1}^{i-2}N_j\sum_{k=l_{i-1,j}+\frac{1}{2}(1+\gamma_{i-1,j})}^{l_{i,j}+\frac{1}{2}(\gamma_{i,j}-1)}\frac{{\Delta x_k}^3}{\Delta x_i+\Delta x_{i-1}}\frac{\partial}{\partial x'}\{K(x_k,x_j)n(t,x_k)\}+\mathcal{O}(\Delta x^3).
\end{aligned}$$

Thus, we have

$$\begin{aligned}
I_4 =& \frac{1}{2}\sum_{j=1}^{i-2}N_j\int_{x_{i-1}-x_j}^{x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}}\lambda_i^-(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-2}N_j\sum_{x_{i-1}\le x_j+x_k<x_i}\lambda_i^-(x_k+x_j)K(x_k,x_j)N_k \\
&+ \frac{1}{2}\sum_{j=1}^{i-2}N_j\int_{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}}^{x_i-x_j}\lambda_i^-(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{12}\sum_{j=1}^{i-2}N_j\sum_{k=l_{i-1,j}+\frac{1}{2}(1+\gamma_{i-1,j})}^{l_{i,j}+\frac{1}{2}(\gamma_{i,j}-1)}\frac{{\Delta x_k}^3}{\Delta x_i+\Delta x_{i-1}}\frac{\partial}{\partial x'}\{K(x_k,x_j)n(t,x_k)\}+\mathcal{O}(\Delta x^3).
\end{aligned} \tag{5.28}$$

The integrals I_2 and I_5.

Now we consider the second term

$$I_2 = \frac{1}{2}\int_{x_{i-1/2}}^{x_i}\int_{x_i}^{x_{i+1}}\lambda_i^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy.$$

Here, we apply the right rectangle rule and get

$$I_2 = \frac{1}{4}\int_{x_i}^{x_{i+1}}\lambda_i^+(x)K(x-x_i,x_i)n(t,x-x_i)n(t,x_i)\Delta x_i dx+\mathcal{O}(\Delta x^3).$$

The above integral on the right hand side can be rewritten as

$$\begin{aligned}I_2 =& \frac{1}{2}\int_{x_i}^{x_{i+1}} \lambda_i^+(x) K(x-x_i, x_i) n(t, x-x_i) N_i dx \\ &- \frac{1}{4}\int_{x_i}^{x_{i+1}} \lambda_i^+(x) K(x-x_i, x_i) n(t, x-x_i) N_i dx + \mathcal{O}(\Delta x^3).\end{aligned}$$

We apply the left rectangle rule in the second integral on the right hand side and use $K(0, x_i) = 0$ which gives us a third order term. Therefore, we obtain

$$I_2 = \frac{1}{2}\int_{x_i}^{x_{i+1}} \lambda_i^+(x) K(x-x_i, x_i) n(t, x-x_i) N_i dx + \mathcal{O}(\Delta x^3).$$

Using the substitution $x - x_i = x'$, we get

$$\begin{aligned}I_2 =& \frac{1}{2}N_i \int_0^{x_{i+1}-x_i} \lambda_i^+(x'+x_i) K(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3), \\ =& \frac{1}{2}N_i \sum_{k=1}^{l_{i+1,i}+\frac{1}{2}(\gamma_{i+1,i}-1)} \int_{x_{k-1/2}}^{x_{k+1/2}} \lambda_i^+(x'+x_i) K(x', x_i) n(t, x') dx' \\ &+ \frac{1}{2}N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1}-x_i} \lambda_i^+(x'+x_i) K(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3).\end{aligned}$$

Using the midpoint rule around x_k in the first term on the right hand side, we obtain

$$\begin{aligned}I_2 =& \frac{1}{2}N_i \sum_{k=1}^{l_{i+1,i}+\frac{1}{2}(\gamma_{i+1,i}-1)} \lambda_i^+(x_k+x_i) K(x_k, x_i) n(t, x_k) \Delta x_k \\ &+ \frac{1}{2}N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1}-x_i} \lambda_i^+(x'+x_i) K(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3).\end{aligned}$$

This can be further rewritten as

$$\begin{aligned}I_2 =& \frac{1}{2}N_i \sum_{x_i+x_k<x_{i+1}} \lambda_i^+(x_k+x_i) K(x_k, x_i) N_k(t) \\ &+ \frac{1}{2}N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1}-x_i} \lambda_i^+(x'+x_i) K(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3). \qquad (5.29)\end{aligned}$$

Before combining all these integrals together, we have to discretize the integral I_5 also. Let us finally consider

$$I_5 = \frac{1}{2}\int_{x_{i-3/2}}^{x_{i-1}} \int_{x_{i-1}}^{x_i} \lambda_i^-(x) K(x-y, y) n(t, x-y) n(t, y) dx dy.$$

Similarly as before in I_2, we obtain

$$\begin{aligned}I_5 =& \frac{1}{2}N_{i-1} \sum_{k=1}^{l_{i,i-1}+\frac{1}{2}(\gamma_{i,i-1}-1)} \lambda_i^-(x_k + x_{i-1})K(x_k, x_{i-1})n(t, x_k)\Delta x_k \\ &+ \frac{1}{2}N_{i-1} \int_{x_{l_{i,i-1}+\frac{1}{2}\gamma_{i,i-1}}}^{x_i - x_{i-1}} \lambda_i^-(x' + x_{i-1})K(x', x_{i-1})n(t, x')dx' + \mathcal{O}(\Delta x^3).\end{aligned}$$

The integral terms on the right hand side can be rewritten as

$$\begin{aligned}I_5 =& \frac{1}{2}N_{i-1} \sum_{x_{i-1}+x_k<x_i} \lambda_i^-(x_k + x_{i-1})K(x_k, x_{i-1})N_k(t) \\ &+ \frac{1}{2}N_{i-1} \int_{x_{l_{i,i-1}+\frac{1}{2}\gamma_{i,i-1}}}^{x_i - x_{i-1}} \lambda_i^-(x' + x_{i-1})K(x', x_{i-1})n(t, x')dx' + \mathcal{O}(\Delta x^3). \qquad (5.30)\end{aligned}$$

Collecting together (5.23), (5.24), (5.27), (5.28), (5.29), (5.30) and substituting all these terms into equation (5.20), we obtain

$$\begin{aligned}B_i =& \sum_{x_i \le x_j + x_k < x_{i+1}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\lambda_i^+(x_k + x_j)K(x_k, x_j)N_jN_k \\ &+ \sum_{x_{i-1} \le x_j + x_k < x_i}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\lambda_i^-(x_k + x_j)K(x_k, x_j)N_jN_k \\ &+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i - x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x' + x_j)K(x', x_j)n(t, x')dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1} - x_j} \lambda_i^+(x' + x_j)K(x', x_j)n(t, x')dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i-2} N_j \int_{x_{i-1} - x_j}^{x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}} \lambda_i^-(x' + x_j)K(x', x_j)n(t, x')dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}}^{x_i - x_j} \lambda_i^-(x' + x_j)K(x', x_j)n(t, x')dx' \\ &- \frac{1}{12}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{\Delta x_k{}^3}{\Delta x_i + \Delta x_{i+1}} \frac{\partial}{\partial x'}\{K(x_k, x_j)n(t, x_k)\} \\ &+ \frac{1}{12}\sum_{j=1}^{i-2} N_j \sum_{k=l_{i-1,j}+\frac{1}{2}(1+\gamma_{i-1,j})}^{l_{i,j}+\frac{1}{2}(\gamma_{i,j}-1)} \frac{\Delta x_k{}^3}{\Delta x_i + \Delta x_{i-1}} \frac{\partial}{\partial x'}\{K(x_k, x_j)n(t, x_k)\} + \mathcal{O}(\Delta x^3) + \mathfrak{J}_i(f).\end{aligned}$$

The first two terms on the right hand side are exactly the fixed pivot discretization $\hat{B}_i^{FP}$ from (5.12). Therefore, we have

$$\begin{aligned}
B_i =& \hat{B}_i^{FP} + \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1}-x_j} \lambda_i^+(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-2} N_j \int_{x_{i-1}-x_j}^{x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}} \lambda_i^-(x'+x_j)K(x',x_j)n(t,x')dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}}^{x_i-x_j} \lambda_i^-(x'+x_j)K(x',x_j)n(t,x')dx' \\
&- \frac{1}{12}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} \frac{\partial}{\partial x'}\{K(x_k,x_j)n(t,x_k)\} \\
&+ \frac{1}{12}\sum_{j=1}^{i-2} N_j \sum_{k=l_{i-1,j}+\frac{1}{2}(1+\gamma_{i-1,j})}^{l_{i,j}+\frac{1}{2}(\gamma_{i,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} \frac{\partial}{\partial x'}\{K(x_k,x_j)n(t,x_k)\} + \mathcal{O}(\Delta x^3) + \mathfrak{J}_i(f).
\end{aligned} \tag{5.31}$$

Let us denote the sum of first four integrals and the difference of remaining two terms on the right hand side by E and E', respectively.
Finally, equation (5.31) can be written as

$$B_i = \hat{B}_i^{FP} + E + E' + \mathcal{O}(\Delta x^3) + \mathfrak{J}_i(f).$$

After substituting $\mathfrak{J}_i(f)$ we get for $i = 2, \ldots, I-1$

$$\begin{aligned}
B_i =& \hat{B}_i^{FP} + E + E' + \frac{f(x_i)}{2}\left[\Delta x_i - \left(\frac{\Delta x_{i-1} + \Delta x_{i+1}}{2}\right)\right] \\
&- \frac{f'(x_i)}{12}\left[(\Delta x_{i+1} - \Delta x_{i-1})\left\{\Delta x_i + \left(\frac{\Delta x_{i-1} + \Delta x_{i+1}}{2}\right)\right\}\right] + \mathcal{O}(\Delta x^3).
\end{aligned} \tag{5.32}$$

Birth term on boundary cells

Now we evaluate the order of the birth term on boundary cells. First we consider the birth term for $i = 1$

$$B_1 = \frac{1}{2}\int_{x_{1-1/2}}^{x_{1+1/2}} \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx.$$

Using the Lemma 5.3.1, the birth term can be rewritten as

$$B_1 = \frac{1}{2}\int_{x_1}^{x_2} \lambda_1^+(x)\int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx + \mathfrak{J}_1(f).$$

Changing the order of integration we get

$$\begin{aligned}B_1 =& \frac{1}{2}\int_0^{x_1}\int_{x_1}^{x_2} \lambda_1^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\ &+ \frac{1}{2}\int_{x_1}^{x_2}\int_y^{x_2} \lambda_1^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy + \mathfrak{J}_1(f).\end{aligned}$$

This can be further rewritten as

$$\begin{aligned}B_1 =& \frac{1}{2}\int_{x_{1/2}}^{x_1}\int_{x_1}^{x_2} \lambda_1^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\ &+ \frac{1}{2}\int_{x_1}^{x_{1+1/2}}\int_y^{x_2} \lambda_1^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy\\ &+ \frac{1}{2}\int_{x_{1+1/2}}^{x_2}\int_y^{x_2} \lambda_1^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy + \mathfrak{J}_1(f).\end{aligned}$$

We apply the right rectangle rule in outer and inner integrals respectively of the first term as well as in the outer integral of the third term. Both of these terms are of second order separately. Also one uses the left rectangle rule in the outer integral of the second term to get

$$B_1 = \frac{1}{4}\Delta x_1 \int_{x_1}^{x_2} \lambda_1^+(x)K(x-x_1,x_1)n(t,x-x_1)n(t,x_1)dx + \mathcal{O}(\Delta x^2) + \mathfrak{J}_1(f).$$

Again by applying the right rectangle rule we obtain

$$B_1 = \frac{1}{2}N_1 \sum_{x_1+x_k<x_2} \lambda_i^+(x_k+x_1)K(x_k,x_1)N_k + \mathcal{O}(\Delta x^2) + \mathfrak{J}_1(f).$$

In terms of fixed pivot discretization we have

$$B_1 = \hat{B}_1^{FP} + \frac{f(x_1)}{4}[3\Delta x_1 - \Delta x_2] + \mathcal{O}(\Delta x^2). \tag{5.33}$$

From (5.19), we have

$$f(t,x_1) = \frac{1}{2}\int_0^{x_1} K(x_1-y,y)n(t,x_1-y)n(t,y)dy.$$

The application of the right rectangle rule in the above integral gives $f(x_1) = \mathcal{O}(\Delta x)$. Substituting this value of $f(x_1)$ in (5.33), we obtain

$$B_1 = \hat{B}_1^{FP} + \mathcal{O}(\Delta x^2). \tag{5.34}$$

Finally we consider the boundary cell $i = I$

$$B_I = \frac{1}{2}\int_{x_{I-1/2}}^{x_{I+1/2}} \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx.$$

Using the Lemma 5.3.1, the birth term can be rewritten as

$$\begin{aligned} B_I =& \frac{1}{2}\int_{x_I}^{x_{I+1}} \lambda_I^+(x) \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx \\ &+ \frac{1}{2}\int_{x_{I-1}}^{x_I} \lambda_I^-(x) \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx + \mathfrak{J}_I(f). \end{aligned}$$

After changing the order of integration, we get

$$\begin{aligned} B_I =& \frac{1}{2}\int_0^{x_I} \int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\ &+ \frac{1}{2}\int_{x_I}^{x_{I+1}} \int_y^{x_{I+1}} \lambda_I^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\ &+ \frac{1}{2}\int_0^{x_{I-1}} \int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\ &+ \frac{1}{2}\int_{x_{I-1}}^{x_I} \int_y^{x_I} \lambda_I^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy + \mathfrak{J}_I(f). \end{aligned}$$

We split each integral on the right hand side into two parts as

$$
\begin{aligned}
B_I =& \frac{1}{2}\sum_{k=1}^{I-1}\int_{x_{k-1/2}}^{x_{k+1/2}}\int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\int_{x_{I-1/2}}^{x_I}\int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\int_{x_I}^{x_{I+1/2}}\int_{y}^{x_{I+1}} \lambda_I^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\int_{x_{I+1/2}}^{x_{I+1}}\int_{y}^{x_{I+1}} \lambda_I^+(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\sum_{k=1}^{I-2}\int_{x_{k-1/2}}^{x_{k+1/2}}\int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\int_{x_{I-3/2}}^{x_{I-1}}\int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\int_{x_{I-1}}^{x_{I-1/2}}\int_{y}^{x_I} \lambda_I^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy \\
&+ \frac{1}{2}\int_{x_{I-1/2}}^{x_I}\int_{y}^{x_I} \lambda_I^-(x)K(x-y,y)n(t,x-y)n(t,y)dxdy + \mathfrak{I}_I(f).
\end{aligned}
$$

By applying the midpoint, right, left and right rectangle rules to the outer integral of the first and fifth, second and sixth, third and seventh as well as fourth and eighth terms respectively, we obtain

$$
\begin{aligned}
B_I =& \frac{1}{2}\sum_{k=1}^{I-1}\Delta x_k\int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-x_k,x_k)n(t,x-x_k)n(t,x_k)dx + 0 \\
&+ \frac{1}{4}\Delta x_I\int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-x_I,x_I)n(t,x-x_I)n(t,x_I)dx + 0 \\
&+ \frac{1}{2}\sum_{k=1}^{I-2}\Delta x_k\int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-x_k,x_k)n(t,x-x_k)n(t,x_k)dx + 0 \\
&+ \frac{1}{4}\Delta x_{I-1}\int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-x_{I-1},x_{I-1})n(t,x-x_{I-1})n(t,x_{I-1})dx + 0 \\
&+ \mathcal{O}(\Delta x^2) + \mathfrak{I}_I(f).
\end{aligned}
$$

This can be further rewritten as

$$
\begin{aligned}
B_I =& \frac{1}{2}\sum_{k=1}^{I-1} N_k \int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-x_k, x_k)n(t, x-x_k)dx \\
&+ \frac{1}{2}N_I \int_{x_I}^{x_{I+1}} \lambda_I^+(x)K(x-x_I, x_I)n(t, x-x_I)dx \\
&+ \frac{1}{2}\sum_{k=1}^{I-2} N_k \int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-x_k, x_k)n(t, x-x_k)dx \\
&+ \frac{1}{2}N_{I-1} \int_{x_{I-1}}^{x_I} \lambda_I^-(x)K(x-x_{I-1}, x_{I-1})n(t, x-x_{I-1})dx + \mathcal{O}(\Delta x^2) + \mathfrak{J}_I(f).
\end{aligned}
$$

The first, second, third and fourth term on the right hand side can be solved similar to I_1, I_2, I_4 and I_5 respectively. Thus, we obtain

$$
\begin{aligned}
B_I =& \frac{1}{2}\sum_{j=1}^{I-1} N_j \sum_{x_I \le x_j + x_k < x_{I+1}} \lambda_I^+(x_k + x_j)K(x_k, x_j)N_k \\
&+ \frac{1}{2}N_I \sum_{x_I + x_k < x_{I+1}} \lambda_I^+(x_k + x_I)K(x_k, x_I)N_k \\
&+ \frac{1}{2}\sum_{j=1}^{I-2} N_j \sum_{x_{I-1} \le x_j + x_k < x_I} \lambda_I^-(x_k + x_j)K(x_k, x_j)N_k \\
&+ \frac{1}{2}N_{I-1} \sum_{x_{I-1} + x_k < x_I} \lambda_I^-(x_k + x_{I-1})K(x_k, x_{I-1})N_k + \mathcal{O}(\Delta x^2) + \mathfrak{J}_I(f).
\end{aligned}
$$

Hence,

$$
\begin{aligned}
B_I =& \sum_{x_I \le x_j + x_k < x_{I+1}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) \lambda_I^+(x_k + x_j)K(x_k, x_j)N_j N_k \\
&+ \sum_{x_{I-1} \le x_j + x_k < x_I}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) \lambda_I^-(x_k + x_j)K(x_k, x_j)N_j N_k + \mathcal{O}(\Delta x^2) + \mathfrak{J}_I(f).
\end{aligned}
$$

In terms of fixed pivot discretization, we have

$$
B_I = \hat{B}_I^{FP} + \frac{f(x_I)}{4}[\Delta x_I - \Delta x_{I-1}] + \mathcal{O}(\Delta x^2). \tag{5.35}
$$

5.3.2 Order of the death term and summary of all terms

The integrated death is given as follows

$$
D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} K(x, y)n(t, y)n(t, x)dydx.
$$

The application of the midpoint rule in outer integral gives us

$$D_i = \Delta x_i \int_0^{x_{I+1/2}} K(x_i, y) n(t, y) n(t, x_i) dy + \mathcal{O}(\Delta x^3).$$

This can be rewritten as

$$D_i = N_i(t) \sum_{j=1}^{I} \int_{x_{j-1/2}}^{x_{j+1/2}} K(x, y) n(t, y) dy + \mathcal{O}(\Delta x^3)..$$

Again we apply the midpoint rule in the above integral and obtain

$$D_i = N_i(t) \sum_{j=1}^{I} K(x_i, x_j) n(t, x_j) \Delta x_j + \mathcal{O}(\Delta x^3),$$

i.e.

$$D_i = N_i(t) \sum_{j=1}^{I} K(x_i, x_j) N_j(t) + \mathcal{O}(\Delta x^3),$$

Thus, from (5.12) we have

$$D_i = \hat{D}_i^{FP} + \mathcal{O}(\Delta x^3). \tag{5.36}$$

Finally from the equations (5.32), (5.34), (5.35) and (5.36), we can summarize the spatial truncation error $\sigma_i(t) = B_i - D_i - (\hat{B}_i^{FP} - \hat{D}_i^{FP})$ as follows

$$\sigma_1 = \mathcal{O}(\Delta x^2), \tag{5.37}$$

$$\begin{aligned}\sigma_i =& E + E' + \frac{f(x_i)}{2}\left[\Delta x_i - \left(\frac{\Delta x_{i-1} + \Delta x_{i+1}}{2}\right)\right] \\ & - \frac{f'(x_i)}{12}\left[(\Delta x_{i+1} - \Delta x_{i-1})\left\{\Delta x_i + \left(\frac{\Delta x_{i-1} + \Delta x_{i+1}}{2}\right)\right\}\right] \\ & + \mathcal{O}(\Delta x^3), \quad i = 2, \dots, I-1,\end{aligned} \tag{5.38}$$

$$\sigma_I = \frac{f(x_I)}{4}[\Delta x_I - \Delta x_{I-1}] + \mathcal{O}(\Delta x^2), \tag{5.39}$$

where E and E' are defined in (5.31).

5.3.3 Meshes

Now let us consider the following five different types of meshes to calculate the order of local discretization error. We repeat some details from J. Kumar and Warnecke [51].

Uniform mesh

Let us begin with the case of uniform mesh i.e. $\Delta x_i = \Delta x$ and $x_i = (i-1/2)\Delta x$ for any $i = 1, \ldots, I$. To estimate $\sigma_i(t)$, first we have to evaluate the order of E and E'. In case of uniform grids, we have

$$x_i - x_j = (i-1/2)\Delta x - (j-1/2)\Delta x = (i-j)\Delta x = x_{i-j+1/2},$$

$$x_{i+1} - x_j = (i+1/2)\Delta x - (j-1/2)\Delta x = (i-j+1)\Delta x = x_{i-j+3/2},$$

and

$$x_{i-1} - x_j = (i-3/2)\Delta x - (j-1/2)\Delta x = (i-j-1)\Delta x = x_{i-j-1/2}.$$

By using the definition of indices in (5.26), one can obtain

$$x_i - x_j = x_{i-j+1/2} \in \Lambda_{l_{i,j}}.$$

This implies that

$$x_i - x_j = x_{i-j+1/2} = x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}.$$

Similarly, we can easily obtain

$$x_{i+1} - x_j = x_{i-j+3/2} = x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}},$$

and

$$x_{i-1} - x_j = x_{i-j-1/2} = x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}.$$

Therefore, from (5.31) we have $E = 0$. For uniform grids, we can observe from above that $x_{i-1} - x_j$, $x_i - x_j$, and $x_{i+1} - x_j$ are the right end boundaries of adjacent cells, i.e. $l_{i-1,j} = (i-j-1)$th, $l_{i,j} = (i-j)$th and $l_{i+1,j} = (i-j+1)$th cells, respectively. Here $\gamma_{i-1,j} = \gamma_{i,j} = \gamma_{i+1,j} = 1$. Thus, by substituting the values of all these indices in E' defined in (5.31) and using the taylor series expansion we obtain $E = \mathcal{O}(\Delta x^3)$. Finally, from the equations (5.37-5.39) we estimate

$$\sigma_i(t) = \begin{cases} \mathcal{O}(\Delta x^2) & i = 1, I, \\ \mathcal{O}(\Delta x^3) & i = 2, \ldots, I-1. \end{cases}$$

The order of consistency is given by

$$\begin{aligned} \|\sigma(t)\| =& |\sigma_1(t)| + \sum_{i=2}^{I-1} |\sigma_i(t)| + |\sigma_I(t)| \\ =& \mathcal{O}(\Delta x^2). \end{aligned}$$

Thus the method is second order consistent on a uniform mesh.

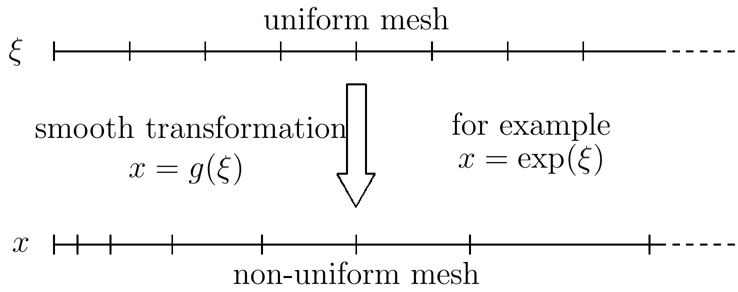


Figure 5.2: Non-uniform smooth mesh.

Non-uniform smooth mesh ($x_{i+1/2} = rx_{i-1/2}$, $r > 1$, $i = 1, \dots, I$)

Suppose, grids to be smooth such that $\Delta x_i - \Delta x_{i-1} = \mathcal{O}(\Delta x^2)$ and $2\Delta x_i - (\Delta x_{i-1} + \Delta x_{i+1}) = \mathcal{O}(\Delta x^3)$, where Δx is the maximum mesh width. This again gives us second order accuracy, which is similar to that of the uniform case. These smooth grids can be obtained by applying some smooth transformation to uniform grids. Let us consider a variable ξ with uniform grids and a smooth transformation $x = g(\xi)$ such that $x_{i\pm1/2} = g(\xi_{i\pm1/2})$ for any $i = 1, \dots, I$ to get non-uniform smooth mesh, see Figure 5.2. Let h be the uniform mesh width in the variable ξ. In case of smooth grids, Taylor series expansion in the smooth transformation gives us

$$\Delta x_i = x_{i+1/2} - x_{i-1/2} = g(\xi_i + h/2) - g(\xi_i - h/2).$$

By applying the Taylor series expansion we get

$$\Delta x_i = hg'(\xi_i) + \frac{h^3}{24} g''(\xi_i) + \mathcal{O}(h^4).$$

Similarly, we have

$$\Delta x_{i+1} = hg'(\xi_i) + h^2 g''(\xi_i) + \mathcal{O}(h^3),$$

and

$$\Delta x_{i-1} = hg'(\xi_i) - h^2 g''(\xi_i) + \mathcal{O}(h^3).$$

Further, we can easily obtain obtain

$$\Delta x_i - \Delta x_{i-1} = \mathcal{O}(h^2),$$

and

$$2\Delta x_i - (\Delta x_{i-1} + \Delta x_{i+1}) = \mathcal{O}(h^3).$$

The above values help us to simplify the equations (5.37-5.39) and give

$$\sigma_1 = \mathcal{O}(h^2), \quad \sigma_I = \mathcal{O}(h^2) \quad \text{and} \quad \sigma_i = E + E' + \mathcal{O}(h^3).$$

To find the order of σ_i, we have to evaluate E and E' separately. First we consider E from (5.31) and set $f(x,y) := K(x,y)n(t,x)$. Then we can write

$$\begin{aligned}
E =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_i - x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j) f(x',x_j)dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1}-x_j} \lambda_i^+(x'+x_j) f(x',x_j)dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-2} N_j \int_{x_{i-1} - x_j}^{x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}} \lambda_i^-(x'+x_j) f(x',x_j)dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}}^{x_i-x_j} \lambda_i^-(x'+x_j) f(x',x_j)dx'.
\end{aligned}$$

Applying the left rectangle rule in first and third integrals and the right rectangle rule in second and fourth integrals, we obtain

$$\begin{aligned}
E =& \frac{1}{4}\sum_{j=1}^{i-1} N_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2}{x_i - x_{i+1}} f(x_i - x_j, x_j) \\
&- \frac{1}{4}\sum_{j=1}^{i} N_j \frac{(x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}} - x_{i+1} + x_j)^2}{x_i - x_{i+1}} f(x_{i+1} - x_j, x_j) \\
&+ \frac{1}{4}\sum_{j=1}^{i-2} N_j \frac{(x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}} - x_{i-1} + x_j)^2}{x_i - x_{i-1}} f(x_{i-1} - x_j, x_j) \\
&- \frac{1}{4}\sum_{j=1}^{i-1} N_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2}{x_i - x_{i-1}} f(x_i - x_j, x_j) + \text{higher order terms.}
\end{aligned}$$

Then we approximate f at $(x_i - x_j, x_j)$ by f evaluated at $(x_{i+1} - x_j, x_j)$ of first and fourth terms, respectively to get

$$\begin{aligned}
E =& \frac{1}{4}\sum_{j=1}^{i-1} N_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2}{x_i - x_{i+1}} \{f(x_{i+1} - x_j, x_j) + (x_i - x_{i+1}) f_{x'}(x_{i+1} - x_j, x_j)\} \\
&- \frac{1}{4}\sum_{j=1}^{i} N_j \frac{(x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}} - x_{i+1} + x_j)^2}{x_i - x_{i+1}} f(x_{i+1} - x_j, x_j) \\
&+ \frac{1}{4}\sum_{j=1}^{i-2} N_j \frac{(x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}} - x_{i-1} + x_j)^2}{x_i - x_{i-1}} f(x_{i-1} - x_j, x_j) \\
&- \frac{1}{4}\sum_{j=1}^{i-1} N_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2}{x_i - x_{i-1}} \{f(x_{i-1} - x_j, x_j) + (x_i - x_{i-1}) f_{x'}(x_{i-1} - x_j, x_j)\} \\
&+ \text{higher order terms.}
\end{aligned}$$

Again approximating $f_{x'}$ at point $(x_{i+1}-x_j, x_j)$ by $f_{x'}$ evaluated at point $(x_{i-1}-x_j, x_j)$ in the second term of the first summation, we obtain

$$\begin{aligned}
E =&\frac{1}{4}\sum_{j=1}^{i-1} N_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}-x_i+x_j)^2}{x_i-x_{i+1}}\{f(x_{i+1}-x_j,x_j)+(x_i-x_{i+1})f_{x'}(x_{i-1}-x_j,x_j)\}\\
&-\frac{1}{4}\sum_{j=1}^{i} N_j \frac{(x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}-x_{i+1}+x_j)^2}{x_i-x_{i+1}} f(x_{i+1}-x_j,x_j)\\
&+\frac{1}{4}\sum_{j=1}^{i-2} N_j \frac{(x_{l_{i-1,j}+\frac{1}{2}\gamma_{i-1,j}}-x_{i-1}+x_j)^2}{x_i-x_{i-1}} f(x_{i-1}-x_j,x_j)\\
&-\frac{1}{4}\sum_{j=1}^{i-1} N_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}-x_i+x_j)^2}{x_i-x_{i-1}}\{f(x_{i-1}-x_j,x_j)+(x_i-x_{i-1})f_{x'}(x_{i-1}-x_j,x_j)\}\\
&+\text{higher order terms.}
\end{aligned}$$

Then we replace j by $j+1$ and $j-1$ respectively in first and third terms. We suppress the dependence on t because it is not explicitly needed. Further we can use the relationship $N_j = n(x_j)\Delta x_j + \mathcal{O}(\Delta x^3)$ for the midpoint rule to obtain

$$\begin{aligned}
E =&\frac{1}{4}\sum_{j=1}^{i-1} n(x_{j+1})\Delta x_{j+1} \frac{(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}}-x_{i+1}+x_{j+1})^2}{x_{i+1}-x_i} f(x_{i+1}-x_{j+1},x_{j+1})\\
&-\frac{1}{4}\sum_{j=1}^{i-1} n(x_j)\Delta x_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}-x_i+x_j)^2}{x_{i+1}-x_i} f(x_{i+1}-x_j,x_j)\\
&+\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1} \frac{(x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}}-x_{i-1}+x_{j-1})^2}{x_i-x_{i-1}} f(x_{i-1}-x_{j-1},x_{j-1})\\
&-\frac{1}{4}\sum_{j=1}^{i-1} n(x_j)\Delta x_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}-x_i+x_j)^2}{x_i-x_{i-1}} f(x_{i-1}-x_j,x_j)+\text{higher order terms.}
\end{aligned}$$

Approximating the functions $x \mapsto f(x_{i\pm1}-x,x)n(x)$ at point x_j by $f(x_{i\pm1}-x,x)n(x)$ evaluated at point $x_{j\pm1}$ of the second and fourth sums on the right hand side respectively, we get

$$\begin{aligned}
E = &\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j+1})\Delta x_{j+1}\frac{(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2}{x_{i+1}-x_i} f(x_{i+1}-x_{j+1}, x_{j+1})\\
&-\frac{1}{4}\sum_{j=2}^{i-1} \Delta x_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2}{x_{i+1}-x_i}\Big\{ n(x_{j+1})f(x_{i+1}-x_{j+1}, x_{j+1})\\
&\qquad + (x_j - x_{j+1})\frac{\partial}{\partial x'}\{n(x_{j+1})f(x_{i+1}-x_{j+1}, x_{j+1})\}\Big\}\\
&+\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1}\frac{(x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2}{x_i - x_{i-1}} f(x_{i-1}-x_{j-1}, x_{j-1})\\
&-\frac{1}{4}\sum_{j=2}^{i-1} \Delta x_j \frac{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2}{x_i - x_{i-1}}\Big\{ n(x_{j-1})f(x_{i-1}-x_{j-1}, x_{j-1})\\
&\qquad + (x_j - x_{j-1})\frac{\partial}{\partial x'}\{n(x_{j-1})f(x_{i-1}-x_{j-1}, x_{j-1})\}\Big\}\\
&\qquad + \text{higher order terms.}
\end{aligned}$$

This can be rewritten as

$$\begin{aligned}
E = &\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j+1})(\Delta x_{j+1} - \Delta x_j)\frac{(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2}{x_{i+1}-x_i} f(x_{i+1}-x_{j+1}, x_{j+1})\\
&+\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j+1})\Delta x_j \frac{f(x_{i+1}-x_{j+1}, x_{j+1})}{x_{i+1}-x_i}\\
&\qquad \times \Big\{ (x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 - (x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 \Big\}\\
&+\frac{1}{4}\sum_{j=2}^{i-1} \Delta x_j \frac{\partial}{\partial x'}\{n(x_{j+1})f(x_{i+1}-x_{j+1}, x_{j+1})\}\frac{(x_{j+1}-x_j)}{x_{i+1}-x_i}(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2\\
&-\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j-1})(\Delta x_j - \Delta x_{j-1})\frac{(x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2}{x_i - x_{i-1}} f(x_{i-1}-x_{j-1}, x_{j-1})\\
&-\frac{1}{4}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_j \frac{f(x_{i-1}-x_{j-1}, x_{j-1})}{x_i - x_{i-1}}\\
&\qquad \times \Big\{ (x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 - (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2 \Big\}\\
&-\frac{1}{4}\sum_{j=2}^{i-1} \Delta x_j \frac{\partial}{\partial x'}\{n(x_{j-1})f(x_{i-1}-x_{j-1}, x_{j-1})\}\frac{(x_j - x_{j-1})}{x_i - x_{i-1}}(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2\\
&\qquad + \text{higher order terms.}
\end{aligned}$$

Let us denote the each sum on the right hand side by $E_1, \dots, E_6$ respectively. Therefore, we have

$$E = E_1 + E_2 + E_3 - E_4 - E_5 - E_6 + \text{higher order terms.} \tag{5.40}$$

In case of smooth grids, it is easy to show that

$$\Delta x_j - \Delta x_{j-1} = \mathcal{O}(\Delta x^2).$$

This implies that $E_4 = \mathcal{O}(\Delta x^2)$. Then by using Taylor's series expansion, we can easily take a second order approximation of E_4. This gives us

$$E_4 = \frac{1}{4}\sum_{j=2}^{i-1} n(x_{j+1}) f(x_{i+1} - x_{j+1}, x_{j+1})(\Delta x_j - \Delta x_{j-1}) \frac{(x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2}{x_i - x_{i-1}} + \mathcal{O}(\Delta x^3).$$

Let us first consider

$$E_1 - E_4 = \frac{1}{2}\sum_{j=2}^{i-1} n(x_{j+1}) f(x_{i+1} - x_{j+1}, x_{j+1}) \times \left\{ \frac{(\Delta x_{j+1} - \Delta x_j)}{\Delta x_i + \Delta x_{i+1}} (x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 - \frac{(\Delta x_j - \Delta x_{j-1})}{\Delta x_i + \Delta x_{i-1}} (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2 \right\} + \mathcal{O}(\Delta x^3).$$

To prove $E_1 - E_4 = \mathcal{O}(\Delta x^3)$, we have to show that

$$(\Delta x_i + \Delta x_{i-1})(\Delta x_{j+1} - \Delta x_j)(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 \tag{5.41}$$
$$- (\Delta x_i + \Delta x_{i+1})(\Delta x_j - \Delta x_{j-1})(x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2 = \mathcal{O}(\Delta x^6). \tag{5.42}$$

Since h is the uniform mesh width in the variable ξ, we have

$$\Delta x_i = x_{i+1/2} - x_{i-1/2} = g(\xi_i + h/2) - g(\xi_i - h/2).$$

By applying the Taylor series expansion we get

$$\Delta x_i = h g'(\xi_i) + \frac{h^3}{24} g''(\xi_i) + \mathcal{O}(h^4).$$

Similarly, we have

$$\Delta x_{i+1} = h g'(\xi_i) + h^2 g''(\xi_i) + \mathcal{O}(h^3),$$

and

$$\Delta x_{i-1} = hg'(\xi_i) - h^2 g''(\xi_i) + \mathcal{O}(h^3).$$

Further, we have

$$\Delta x_i + \Delta x_{i-1} = 2hg'(\xi_i) - h^2 g''(\xi_i) + \mathcal{O}(h^3), \tag{5.43}$$

and

$$\Delta x_i + \Delta x_{i+1} = 2hg'(\xi_i) + h^2 g''(\xi_i) + \mathcal{O}(h^3). \tag{5.44}$$

Similarly, one can write

$$\Delta x_j - \Delta x_{j-1} = h^2 g''(\xi_j) + \mathcal{O}(h^3),$$

and

$$\Delta x_{j+1} - \Delta x_j = h^2 g''(\xi_j) + \mathcal{O}(h^3).$$

Furthermore, we obtain

$$(\Delta x_i + \Delta x_{i-1})(\Delta x_{j+1} - \Delta x_j) = 2h^3 g'(\xi_i) g''(\xi_j) + \mathcal{O}(h^4), \tag{5.45}$$

and

$$(\Delta x_i + \Delta x_{i+1})(\Delta x_j - \Delta x_{j-1}) = 2h^3 g'(\xi_i) g''(\xi_j) + \mathcal{O}(h^4). \tag{5.46}$$

Let us consider ξ_{11}, ξ_{12}, ξ_{21}, ξ_{22}, ξ_{31} and ξ_{32} are corresponding points on uniform mesh for $x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}}$, $x_{i+1} - x_{j+1}$, $x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}$, $x_i - x_j$, $x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}}$ and $x_{i-1} - x_{j-1}$, respectively.
Here we consider a particular type of non-uniform smooth grids i.e. $x_{i+1/2} = rx_{i-1/2}$, $r > 1, i = 1, \dots I$. Such grids are called as geometric grids. These grids can be obtained by applying exponential function as a smooth transformation. Here we have $x_{i+1/2} = \exp(\xi_{i+1/2}) = \exp(h + \xi_{i-1/2}) = \exp(h)\exp(\xi_{i-1/2}) = \exp(h) x_{i-1/2} =: rx_{i-1/2}$, $r > 1$.
By the definition of the indices in (5.26), we know

$$x_{i+1} - x_{j+1} \in \Lambda_{l_{i+1,j+1}}, \quad x_i - x_j \in \Lambda_{l_{i,j}} \quad \text{and} \quad x_{i-1} - x_{j-1} \in \Lambda_{l_{i-1,j-1}}.$$

For geometric grids, we have

$$x_{i+1} - x_{j+1} = r(x_i - x_j) = r^2(x_{i-1} - x_{j-1}).$$

Therefore, we have

$$l_{i+1,j+1} = l_{i,j} + 1 = l_{i-1,j-1} + 2.$$

Further, in case of geometric grids, we have

$$\gamma_{i+1,j+1} = \gamma_{i,j} = \gamma_{i-1,j-1}.$$

Let us consider

$$\begin{aligned} h_1 = \xi_{11} - \xi_{12} =& \ln(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}}) - \ln(x_{i+1} - x_{j+1}) \\ =& \ln\left(\frac{x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}}}{x_{i+1} - x_{j+1}}\right) = \ln\left(\frac{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}}{x_i - x_j}\right) = \xi_{21} - \xi_{22} \\ =& \ln\left(\frac{x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}}}{x_{i-1} - x_{j-1}}\right) = \xi_{31} - \xi_{32}. \end{aligned}$$

Similarly, we can estimate

$$\xi_{12} - \xi_{32} = \ln\left(\frac{x_{i+1} - x_{j+1}}{x_{i-1} - x_{j-1}}\right) = \ln(r^2) = 2h.$$

By the application of smooth transformation we can write

$$[x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - (x_{i+1} - x_{j+1})]^2 = [g(\xi_{11}) - g(\xi_{12})]^2 = h_1^2\{g'(\xi_{12})\}^2 + \mathcal{O}(h^3), \quad (5.47)$$

and

$$[x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - (x_{i-1} - x_{j-1})]^2 = [g(\xi_{31}) - g(\xi_{32})]^2 = h_1^2\{g'(\xi_{32})\}^2 + \mathcal{O}(h^3). \quad (5.48)$$

Substituting (5.45), (5.46), (5.47) and (5.48) into the left hand side of (5.41), we obtain

$$\begin{aligned} (\Delta x_i + & \Delta x_{i-1})(\Delta x_{j+1} - \Delta x_j)(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 \\ & - (\Delta x_i + \Delta x_{i+1})(\Delta x_j - \Delta x_{j-1})(x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2 \\ =& [2h^3 g'(\xi_i)g''(\xi_j) + \mathcal{O}(h^4)][h_1^2\{g'(\xi_{12})\}^2 + \mathcal{O}(h^3)] \\ & - [2h^3 g'(\xi_i)g''(\xi_j) + \mathcal{O}(h^4)][h_1^2\{g'(\xi_{32})\}^2 + \mathcal{O}(h^3)] \\ =& 2h^3 h_1^2 g'(\xi_i)g''(\xi_j)[\{g'(\xi_{12})\}^2 - \{g'(\xi_{32})\}^2] + \mathcal{O}(h^6) \\ =& 2h^3 h_1^2 g'(\xi_i)g''(\xi_j)[\{g'(\xi_{12})\}^2 - \{g'(\xi_{12} - 2h)\}^2] + \mathcal{O}(h^6) \\ =& - 8h^4 h_1^2 g'(\xi_i)g''(\xi_j)g'(\xi_{12})g''(\xi_{12}) + \mathcal{O}(h^6) = \mathcal{O}(h^6). \end{aligned}$$

This implies that (5.41) holds. Therefore we have

$$E_1 - E_4 = \mathcal{O}(\Delta x^3). \quad (5.49)$$

Let us consider

$$\begin{aligned} E_5 = \frac{1}{2}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_j \frac{f(x_{i-1} - x_{j-1}, x_{j-1})}{\Delta x_i + \Delta x_{i-1}} \\ \times \left\{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 - (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2\right\} \end{aligned}$$

By using smooth transformation and Taylor's series expansions, we have

$$[x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - (x_i - x_j)]^2 = [g(\xi_{21}) - g(\xi_{22})]^2 = h_1^2\{g'(\xi_{22})\}^2 + \mathcal{O}(h^3),$$

and

$$[x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - (x_{i-1} - x_{j-1})]^2 = [g(\xi_{31}) - g(\xi_{32})]^2 = h_1^2\{g'(\xi_{32})\}^2 + \mathcal{O}(h^3).$$

Since

$$\xi_{22} - \xi_{32} = \ln\left(\frac{x_i - x_j}{x_{i-1} - x_{j-1}}\right) = \ln(r) = h.$$

Now let us take

$$\begin{aligned}
[x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - (x_i - x_j)]^2 &- [x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - (x_{i-1} - x_{j-1})]^2 \\
&= h_1^2[\{g'(\xi_{22})\}^2 - \{g'(\xi_{32})\}^2] + \mathcal{O}(h^3) \\
&= h_1^2[\{g'(\xi_{32+h})\}^2 - \{g'(\xi_{32})\}^2] + \mathcal{O}(h^3) \\
&= h_1^2[hg''(\xi_{32})g'(\xi_{32}) + \mathcal{O}(h^2)] + \mathcal{O}(h^3) = \mathcal{O}(h^3).
\end{aligned}$$

This implies that $E_5 = \mathcal{O}(\Delta x^2)$. Then by using Taylor's series expansion, we can easily take a second order approximation of E_5. This gives us

$$\begin{aligned}
E_5 = \frac{1}{2}\sum_{j=2}^{i-1} n(x_{j+1})\Delta x_j \frac{f(x_{i+1} - x_{j+1}, x_{j+1})}{\Delta x_i + \Delta x_{i-1}} \\
\times \left\{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 - (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2\right\} + \mathcal{O}(\Delta x^3)
\end{aligned}$$

Now let us consider

$$\begin{aligned}
E_2 - E_5 =& \frac{1}{2}\sum_{j=2}^{i-1} n(x_{j+1})\Delta x_j f(x_{i+1} - x_{j+1}, x_{j+1}) \\
&\times \left[\frac{1}{\Delta x_i + \Delta x_{i+1}}\left\{(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 - (x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2\right\}\right. \\
&\left. - \frac{1}{\Delta x_i + \Delta x_{i-1}}\left\{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 - (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2\right\}\right] \\
&+ \mathcal{O}(\Delta x^3).
\end{aligned}$$

To prove that $E_2 - E_5 = \mathcal{O}(\Delta x^3)$, we need to show that

$$\begin{aligned}
(\Delta x_i + \Delta x_{i-1})\left\{(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 - (x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2\right\} \\
-(\Delta x_i + \Delta x_{i+1})\left\{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 - (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2\right\} \\
= \mathcal{O}(\Delta x^5). \qquad (5.50)
\end{aligned}$$

By using smooth transformation and Taylor's series expansions, we have

$$\begin{aligned}[x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - (x_{i+1} - x_{j+1})]^2 &= [g(\xi_{11}) - g(\xi_{12})]^2 \\ &= h_1^2\{g'(\xi_{12})\}^2 + h_1^3 g'(\xi_{12})g''(\xi_{12}) + \mathcal{O}(h^4),\end{aligned}$$

$$\begin{aligned}[x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - (x_i - x_j)]^2 &= [g(\xi_{21}) - g(\xi_{22})]^2 \\ &= h_1^2\{g'(\xi_{22})\}^2 + h_1^3 g'(\xi_{22})g''(\xi_{22}) + \mathcal{O}(h^4),\end{aligned}$$

and

$$\begin{aligned}[x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - (x_{i-1} - x_{j-1})]^2 &= [g(\xi_{31}) - g(\xi_{32})]^2 \\ &= h_1^2\{g'(\xi_{32})\}^2 + +h_1^3 g'(\xi_{32})g''(\xi_{32}) + \mathcal{O}(h^4).\end{aligned}$$

Since

$$\begin{aligned}\xi_{12} - \xi_{22} &= \ln\left(\frac{x_{i+1} - x_{j+1}}{x_i - x_j}\right) = \ln(r) = h \\ &= \ln\left(\frac{x_i - x_j}{x_{i-1} - x_{j-1}}\right) = \xi_{22} - \xi_{32}.\end{aligned}$$

We substitute of all these values in the left hand side of (5.50) and use Taylor's series expansions to get

$$\begin{aligned}&(\Delta x_i + \Delta x_{i-1})\left\{(x_{l_{i+1,j+1}+\frac{1}{2}\gamma_{i+1,j+1}} - x_{i+1} + x_{j+1})^2 - (x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2\right\} \\ &\quad - (\Delta x_i + \Delta x_{i+1})\left\{(x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2 - (x_{l_{i-1,j-1}+\frac{1}{2}\gamma_{i-1,j-1}} - x_{i-1} + x_{j-1})^2\right\} \\ &= [hg'(\xi_i) + \mathcal{O}(h^2)] \\ &\quad \times \left[h_1^2\{(g'(\xi_{12}))^2 - (g'(\xi_{22}))^2\} + h_1^3\{g'(\xi_{12})g''(\xi_{12}) - g'(\xi_{22})g''(\xi_{22})\} + \mathcal{O}(h^4)\right] \\ &\quad - [hg'(\xi_i) + \mathcal{O}(h^2)] \\ &\quad \times \left[h_1^2\{(g'(\xi_{22}))^2 - (g'(\xi_{32}))^2\} + h_1^3\{g'(\xi_{22})g''(\xi_{22}) - g'(\xi_{32})g''(\xi_{32})\} + \mathcal{O}(h^4)\right] \\ &= [hg'(\xi_i) + \mathcal{O}(h^2)] \\ &\quad \times \left[2hh_1^2 g'(\xi_{22})g''(\xi_{22}) + h_1^3\left\{h\{(g''(\xi_{22}))^2 + g'(\xi_{22})g'''(\xi_{22})\}\right\} + \mathcal{O}(h^4)\right] \\ &\quad - [hg'(\xi_i) + \mathcal{O}(h^2)] \\ &\quad \times \left[2hh_1^2 g'(\xi_{22})g''(\xi_{22}) + h_1^3\left\{h\{(g''(\xi_{22}))^2 + g'(\xi_{22})g'''(\xi_{22})\}\right\} + \mathcal{O}(h^4)\right] \\ &= 2h^2h_1^2 g'(\xi_{22})g''(\xi_{22}) - 2h^2h_1^2 g'(\xi_{22})g''(\xi_{22}) + \mathcal{O}(h^5) = \mathcal{O}(h^5).\end{aligned}$$

This shows that (5.50) holds. Therefore, we have

$$E_2 - E_5 = \mathcal{O}(\Delta x^3). \tag{5.51}$$

Finally, by using the application of Taylor's series expansion in E_6 we consider

$$E_3 - E_6 = \frac{1}{4}\sum_{j=2}^{i-1} \Delta x_j \frac{\partial}{\partial x'}\{n(x_{j+1})f(x_{i+1} - x_{j+1}, x_{j+1})\}$$
$$\left[\frac{\Delta x_j + \Delta x_{j+1}}{\Delta x_i + \Delta x_{i+1}} - \frac{\Delta x_j + \Delta x_{j-1}}{\Delta x_i + \Delta x_{i-1}}\right](x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}} - x_i + x_j)^2.$$

To prove that $E_3 - E_6 = \mathcal{O}(\Delta x^3)$, one has to show that

$$(\Delta x_i + \Delta x_{i-1})(\Delta x_j + \Delta x_{j+1}) - (\Delta x_i + \Delta x_{i+1})(\Delta x_j + \Delta x_{j-1}) = \mathcal{O}(\Delta x^3). \tag{5.52}$$

By applying the smooth transformation and Taylor's series expansion, we have

$$\Delta x_j + \Delta x_{j-1} = 2hg'(\xi_j) - h^2 g''(\xi_j) + \mathcal{O}(h^3),$$

and

$$\Delta x_i + \Delta x_{i+1} = 2hg'(\xi_j) + h^2 g''(\xi_j) + \mathcal{O}(h^3).$$

Furthermore, we obtain

$$(\Delta x_i + \Delta x_{i-1})(\Delta x_j + \Delta x_{j+1}) = 4h^2 g'(\xi_i)g'(\xi_j) + \mathcal{O}(h^3), \tag{5.53}$$

and

$$(\Delta x_i + \Delta x_{i+1})(\Delta x_j + \Delta x_{j-1}) = 4h^2 g'(\xi_i)g'(\xi_j) + \mathcal{O}(h^3). \tag{5.54}$$

Equations (5.53), (5.54) implies that (5.52) holds. Therefore, we have

$$E_3 - E_6 = \mathcal{O}(\Delta x^3). \tag{5.55}$$

Finally, we substitute (5.49), (5.51) and (5.55) into (5.40) to obtain

$$E = \mathcal{O}(\Delta x^3).$$

Now let us consider E' from (5.31) and set $f_x(x, y) := \frac{\partial}{\partial x}\{K(x, y)n(t, x)\}$. Then we can write

$$E' = -\frac{1}{12}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} f_{x'}(x_k, x_j)$$
$$+ \frac{1}{12}\sum_{j=1}^{i-2} N_j \sum_{k=l_{i-1,j}+\frac{1}{2}(1+\gamma_{i-1,j})}^{l_{i,j}+\frac{1}{2}(\gamma_{i,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} f_{x'}(x_k, x_j).$$

We replace j by $j-1$ in the second term on the right hand side to get

$$\begin{aligned}
E' =& -\frac{1}{12}\sum_{j=2}^{i-1} n(x_j)\Delta x_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} f_{x'}(x_k, x_j) \\
&+ \frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1} \sum_{k=l_{i-1,j-1}+\frac{1}{2}(1+\gamma_{i-1,j-1})}^{l_{i,j-1}+\frac{1}{2}(\gamma_{i,j-1}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} f_{x'}(x_k, x_{j-1}).
\end{aligned}$$

The application of Taylor's series expansion about $x_j = x_{j-1}$ in $n(x_j)f_{x'}(x_k, x_j)$ of the first term on the right hand side gives

$$\begin{aligned}
E' =& -\frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_j \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} f_{x'}(x_k, x_{j-1}) \\
&+ \frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1} \sum_{k=l_{i-1,j-1}+\frac{1}{2}(1+\gamma_{i-1,j-1})}^{l_{i,j-1}+\frac{1}{2}(\gamma_{i,j-1}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} f_{x'}(x_k, x_{j-1}) + \mathcal{O}(\Delta x^3).
\end{aligned}$$

This can be rewritten as

$$\begin{aligned}
E' =& \frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})(\Delta x_{j-1} - \Delta x_j) \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} f_{x'}(x_k, x_{j-1}) \\
&- \frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1} \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} f_{x'}(x_k, x_{j-1}) \\
&+ \frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1} \sum_{k=l_{i-1,j-1}+\frac{1}{2}(1+\gamma_{i-1,j-1})}^{l_{i,j-1}+\frac{1}{2}(\gamma_{i,j-1}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} f_{x'}(x_k, x_{j-1}) + \mathcal{O}(\Delta x^3).
\end{aligned}$$

For smooth grids, it is easy to show that $\Delta_{j-1} - \Delta x_j = \mathcal{O}(\Delta x^2)$. Therefore, the first term on the right hand side of the above equation is of third order. By using the Taylor series expansion about $x_k = x_j$ in $f_{x'}(x_k, x_{j-1})$ in the remaining terms on right hand side, the above equation can be further rewritten as

$$\begin{aligned}
E' = \frac{1}{12}\sum_{j=2}^{i-1} n(x_{j-1})\Delta x_{j-1} \Bigg[& \sum_{k=l_{i-1,j-1}+\frac{1}{2}(1+\gamma_{i-1,j-1})}^{l_{i,j-1}+\frac{1}{2}(\gamma_{i,j-1}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} \\
& - \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} \Bigg] f_{x'}(x_j, x_{j-1}) + \mathcal{O}(\Delta x^3).
\end{aligned}$$

To prove $E' = \mathcal{O}(\Delta x^3)$, we need to show that

$$\sum_{k=l_{i-1,j-1}+\frac{1}{2}(1+\gamma_{i-1,j-1})}^{l_{i,j-1}+\frac{1}{2}(\gamma_{i,j-1}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} - \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} = \mathcal{O}(\Delta x^3). \tag{5.56}$$

For non-uniform smooth grids of the type $(x_{i+1/2} = r x_{i-1/2},\ r > 1,\ i = 1, \ldots, I$, we have

$$x_{i+1} - x_j = r(x_i - x_{j-1}) \text{ and } x_{i+1} - x_j \in \Lambda_{l_{i+1,j}}, \quad x_i - x_{j-1} \in \Lambda_{l_{i,j-1}}.$$

Therefore, we obtain

$$l_{i+1,j} = l_{i,j-1} + 1.$$

Similarly, one can get

$$l_{i,j} = l_{i-1,j-1} + 1.$$

In case of such smooth grids, it can easily be seen that $\gamma_{i-1,j-1} = \gamma_{i,j}$ and $\gamma_{i,j-1} = \gamma_{i+1,j}$. Let $k_1 := l_{i-1,j-1} + \frac{1}{2}(1 + \gamma_{i-1,j-1})$, $k_2 := l_{i,j} + \frac{1}{2}(1 + \gamma_{i,j}) = k_1 + 1$, $\ldots$, $k_p := l_{i,j-1} + \frac{1}{2}(\gamma_{i,j-1} - 1) = k_{p-1} + 1$, $K_{p+1} := l_{i+1,j} + \frac{1}{2}(\gamma_{i+1,j} - 1) = k_p + 1$. Then the left hand side of (5.56) can be written as

$$\begin{aligned}
&\sum_{k=l_{i-1,j-1}+\frac{1}{2}(1+\gamma_{i-1,j-1})}^{l_{i,j-1}+\frac{1}{2}(\gamma_{i,j-1}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i-1}} - \sum_{k=l_{i,j}+\frac{1}{2}(1+\gamma_{i,j})}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \frac{{\Delta x_k}^3}{\Delta x_i + \Delta x_{i+1}} \\
&= \left[\frac{{\Delta x_{k_1}}^3}{\Delta x_i + \Delta x_{i-1}} - \frac{{\Delta x_{k_2}}^3}{\Delta x_i + \Delta x_{i+1}}\right] + \ldots \\
&\qquad + \left[\frac{{\Delta x_{k_p}}^3}{\Delta x_i + \Delta x_{i-1}} - \frac{{\Delta x_{k_{p+1}}}^3}{\Delta x_i + \Delta x_{i+1}}\right] \\
&= \sum_{m=1}^{p} \left[\frac{{\Delta x_{k_m}}^3}{\Delta x_i + \Delta x_{i-1}} - \frac{{\Delta x_{k_{m+1}}}^3}{\Delta x_i + \Delta x_{i+1}}\right]
\end{aligned}$$

where $k_{m+1} = k_m + 1$. To show that (5.56) holds, one has to prove that

$$(\Delta x_i + \Delta x_{i+1})\Delta x_{k_m}^3 - (\Delta x_i + \Delta x_{i-1})\Delta x_{k_{m+1}}^3 = \mathcal{O}(\Delta x^5). \tag{5.57}$$

Let ξ_{m1}, ξ_{m2}, ξ_{m3} are the corresponding points on the uniform mesh for $x_{k_m+3/2}$, $x_{k_m+1/2}$ and $x_{k_m-1/2}$, respectively. Since

$$\begin{aligned}
\xi_{m1} - \xi_{m2} &= \ln\left(\frac{x_{k_m+3/2}}{x_{k_m+1/2}}\right) = \ln(r) = h \\
&= \ln\left(\frac{x_{k_m+1/2}}{x_{k_m-1/2}}\right) = \xi_{m2} - \xi_{m3}.
\end{aligned}$$

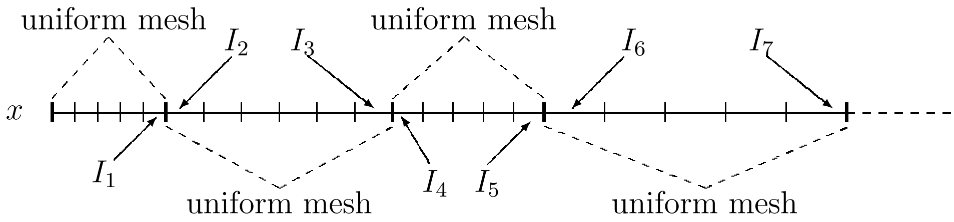


Figure 5.3: Locally uniform smooth mesh.

Then by using smooth transformation and Taylor's series expansion, we can write

$$\begin{aligned}
&(\Delta x_i + \Delta x_{i+1})\Delta x_{k_m}^3 - (\Delta x_i + \Delta x_{i-1})\Delta x_{k_{m+1}}^3 \\
&\quad = [2hg'(\xi_i) + \mathcal{O}(h^2)] \times [g(\xi_{m2}) - g(\xi_{m3})]^3 - [2hg'(\xi_i) + \mathcal{O}(h^2)] \times [g(\xi_{m1}) - g(\xi_{m2})]^3 \\
&\quad = [2hg'(\xi_i) + \mathcal{O}(h^2)] \times [hg'(\xi_{m2}) + \mathcal{O}(h^2)]^3 - [2hg'(\xi_i) + \mathcal{O}(h^2)] \times [hg'(\xi_{m2}) + \mathcal{O}(h^2)]^3 \\
&\quad = 2h^4 g'(\xi_i)[g'(\xi_{m2})]^3 - 2h^4 g'(\xi_i)[g'(\xi_{m2})]^3 + \mathcal{O}(h^5) = \mathcal{O}(h^5).
\end{aligned}$$

This implies that (5.57) holds. Therefore, we have

$$E' = \mathcal{O}(\Delta x^3).$$

This gives us

$$\sigma_i = \mathcal{O}(h^3).$$

Finally, analogous to the uniform mesh, the technique is second order consistent.

Locally uniform mesh

Figure 5.3 explains an example of a locally uniform mesh. First, the computational domain is split into many finite sub-domains and each sub-domain is further split into an equal size mesh. This yields us a locally uniform mesh. It is not easy to find the order of consistency on locally uniform mesh from analysis. So we calculate it later numerically. In this case, the scheme gives only first order consistency.

Oscillatory mesh

A mesh is known to be an oscillatory mesh, if for any $r \neq 1 > 0$, it is given as

$$\Delta x_{i+1} := \begin{cases} r\Delta x_i & \text{if } i \text{ is odd,} \\ \frac{1}{r}\Delta x_i & \text{if } i \text{ is even.} \end{cases}$$

Since there is no cancelation in the leading error terms of equations (5.37-5.39) as well as $E = \mathcal{O}(\Delta x)$ and $E' = \mathcal{O}(\Delta x^2)$ we have

$$\sigma_i(t) = \mathcal{O}(\Delta x), \quad i = 1, \ldots, I, \quad \text{and} \quad \|\sigma(t)\| = \mathcal{O}(1).$$

Thus the fixed pivot method is unfortunately inconsistent on oscillatory meshes. This type of mesh was not considered in J. Kumar and Warnecke [51] and [52] for breakage problems. We have repeated such meshes on the local discretization error obtained in the above mentioned papers. We observed that the fixed pivot method is inconsistent on such meshes and the cell average technique is of first order only. These observations have been also verified numerically.

Non-uniform random mesh

Finally the scheme is examined on non-uniform random grids. Similar to the case of oscillatory mesh, we have $\|\sigma(t)\| = \mathcal{O}(1)$. Thus the method is again inconsistent on non-uniform random meshes.

5.4 Lipschitz conditions on $\hat{\mathbf{B}}(\mathbf{N}(t))$ and $\hat{\mathbf{D}}(\mathbf{N}(t))$

Let us consider the birth term for $0 \le t \le T$ and for all $\mathbf{N}$, $\hat{\mathbf{N}} \in \mathbb{R}^I$

$$\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\hat{\mathbf{N}})\| = \sum_{i=1}^{I} |\hat{B}_i(\mathbf{N}) - \hat{B}_i(\hat{\mathbf{N}})|.$$

Using $K_{j,k} \le C$ from (5.13) and $0 \le \lambda_i^{\pm}(x) \le 1$ from the definition in (5.11), we obtain from (5.12)

$$\begin{aligned}\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\hat{\mathbf{N}})\| \le & \frac{1}{2}C\sum_{i=1}^{I}\sum_{j=1}^{i}\sum_{x_i \le x_j + x_k < x_{i+1}} |N_jN_k - \hat{N}_j\hat{N}_k| \\ & + \frac{1}{2}C\sum_{i=1}^{I}\sum_{j=1}^{i-1}\sum_{x_{i-1} \le x_j + x_k < x_i} |N_jN_k - \hat{N}_j\hat{N}_k| \\ \le & C\sum_{j=1}^{I}\sum_{k=1}^{I} |N_jN_k - \hat{N}_j\hat{N}_k|.\end{aligned}$$

Now we enjoy a useful equality $N_jN_k - \hat{N}_j\hat{N}_k = \frac{1}{2}[(N_j + \hat{N}_j)(N_k - \hat{N}_k) + (N_j - \hat{N}_j)(N_k + \hat{N}_k)]$ to get

$$\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\hat{\mathbf{N}})\| \le \frac{1}{2}C\sum_{j=1}^{I}\sum_{k=1}^{I}\Big[|(N_j + \hat{N}_j)||(N_k - \hat{N}_k)| + |(N_j - \hat{N}_j)||(N_k + \hat{N}_k)|\Big]. \tag{5.58}$$

It can be easily shown that the total number of particles decreases in a coagulation process, i.e.

$$\sum_{j=1}^{I} N_j \le N_T^0 := \text{Total number of particles which are taken initially.}$$

The equation (5.58) can be rewritten as

$$\begin{aligned}\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\hat{\mathbf{N}})\| &\leq N_T^0 C\Bigg[\sum_{k=1}^{I}|(N_k - \hat{N}_k)| + \sum_{j=1}^{I}|(N_j - \hat{N}_j)|\Bigg] \\ &\leq 2N_T^0 C\|\mathbf{N} - \hat{\mathbf{N}}\|. \end{aligned} \tag{5.59}$$

Now we consider the death term

$$\begin{aligned}\|\hat{\mathbf{D}}(\mathbf{N}) - \hat{\mathbf{D}}(\hat{\mathbf{N}})\| &= \sum_{i=1}^{I}|\hat{D}_i(N) - \hat{D}_i(\hat{N})| \\ &\leq \sum_{i=1}^{I}\sum_{j=1}^{I}K(x_i, x_j)|N_iN_j - \hat{N}_i\hat{N}_j| \\ &\leq C\sum_{i=1}^{I}\sum_{j=1}^{I}|N_iN_j - \hat{N}_i\hat{N}_j|.\end{aligned}$$

Again we use the same equality as before to get

$$\|\hat{\mathbf{D}}(\mathbf{N}) - \hat{\mathbf{D}}(\hat{\mathbf{N}})\| \leq 2N_T^0 C\|\mathbf{N} - \hat{\mathbf{N}}\|. \tag{5.60}$$

So we can apply Theorem 5.2.3 to check the positivity of the solution obtained by the fixed pivot technique.

Proposition 5.4.1. *The numerical solution by the fixed pivot technique is non-negative.*

Proof. The Lipschitz condition on $\hat{\mathbf{F}}(t, \hat{\mathbf{M}})$ can be easily shown by using (5.59), (5.60) and (5.8). The death term $\hat{D}_i$ in (5.12) will become zero when $\hat{M}_i = 0$ and (5.8) gives $\hat{F}_i(t, \hat{\mathbf{M}}) \geq 0$. Thus, the Theorem 5.2.3 directly implies the non-negativity of the solution. □

We need the following Gronwall Lemma to prove the Theorem 5.2.4. A slightly more general result is given in Linz [63]. For completeness we give the short proof.

Lemma 5.4.2. *If* $v(t)$ *satisfies*

$$|v(t)| \leq k\int_0^t |v(\tau)|d\tau + \int_0^t |r(\tau)|d\tau, \tag{5.61}$$

with $k > 0$*,*

$$\max_{0\leq t\leq T}|r(t)| \leq R > 0,$$

then

$$|v(t)| \leq \frac{R}{k}[\exp(kt) - 1]. \tag{5.62}$$

Proof. Let $z(t)$ be the solution of

$$z(t) = k\int_0^t z(\tau)d\tau + tR.$$

Since $z(t)$ is a positive and increasing function of t

$$z(t) \geq k\int_0^t z(\tau)d\tau + \int_0^t |r(\tau)|d\tau,$$

and comparing this with (5.61) we have

$$z(t) \geq |v(t)|.$$

But

$$z(t) = \frac{R}{k}[\exp{(kt)} - 1].$$

and (5.62) follows. □

Proof of Theorem 5.2.4

Using the equations (5.16) and (5.17) we have for $\epsilon(t) = \mathbf{N}(t) - \hat{\mathbf{N}}(t)$

$$\frac{d}{dt}\epsilon(t) = \sigma(t) + (\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\hat{\mathbf{N}})) - (\hat{\mathbf{D}}(\mathbf{N}) - \hat{\mathbf{D}}(\hat{\mathbf{N}})).$$

We then take the norm on both sides to get

$$\frac{d}{dt}\|\epsilon(t)\| \leq \|\sigma(t)\| + \|(\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\hat{\mathbf{N}}))\| + \|(\hat{\mathbf{D}}(\mathbf{N}) - \hat{\mathbf{D}}(\hat{\mathbf{N}}))\|.$$

Integrating with respect to t with $\epsilon(0) = 0$ and using the Lipschitz conditions (5.59)-(5.60) we obtain the estimates

$$\|\epsilon(t)\| \leq \int_0^t \|\sigma(\tau)\|d\tau + 2L\int_0^t \|\epsilon(\tau)\|d\tau.$$

From this it follows by Gronwall's Lemma 5.4.2 that

$$\|\epsilon(t)\| \leq \frac{e_h}{2L}[\exp{(2Lt)} - 1], \tag{5.63}$$

where

$$e_h = \max_{0\leq t\leq T} \|\sigma(t)\|.$$

If the scheme is consistent then $\lim_{h\to 0} e_h = 0$. This completes the proof of the Theorem 5.2.4.

Remark 5.4.3. *The proof of the Theorem 5.2.4 follows a related result by Linz [63].*

5.5 Numerical examples

We now justify our mathematical results on the convergence by taking a few numerical examples where we numerically evaluate the experimental order of convergence (EOC). The detailed comparisons of numerical results of number density and moments with analytical solutions can be found in [54, 47].

Now we have to use a suitable ODE solver to solve the resulting set of ODEs. Integrating the resultant system (5.12) by using a standard ODE routine, for example the ODE45, ODE15S solvers in MATLAB, may lead to negative values for the number density at large size classes. These negative values may lead in consequence to instabilities in the overall computation. Therefore, one should take care of the positivity of the solution by the numerical integration routine. The computation time t is set to as 0.3567 for all cases.

First, we consider the following normally distributed initial condition (NIC)

$$n(0,x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]. \tag{5.64}$$

In addition, we take the following aggregation sum and product kernels

$$K(x,y) = k_0(x+y) \quad \text{and} \quad K(x,y) = k_0 xy. \tag{5.65}$$

Since analytical solutions are not available for the above initial condition and aggregation kernels, we use the following formula in order to calculate the experimental order of convergence

$$\text{EOC} = \ln\left(\frac{\|\hat{\mathbf{N}}_h - \hat{\mathbf{N}}_{h/2}\|}{\|\hat{\mathbf{N}}_{h/2} - \hat{\mathbf{N}}_{h/4}\|}\right) \Big/ \ln(2). \tag{5.66}$$

Here $\hat{\mathbf{N}}_h$ represents the numerical solution on a uniform mesh of width h. The other parameters are $\sigma^2 = 0.01$, $\mu = 1$ and $k_0 = 1$. Now we will calculate the EOC on five different types of uniform and non-uniform meshes.

Let us first calculate the EOC for uniform meshes. For a uniform mesh, we fix the minimum and maximum values of x as 0 and 15, respectively in the numerical computation. The numerical results are shown in Table 5.1. As expected from the mathematical analysis, the numerical results exhibit convergence of second order.

	(a) $K(x, y) = k_0(x + y)$		(b) $K(x, y) = k_0xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0598	-	0.0306	-
240	0.0178	1.75	8.4E-3	1.86
480	5.0E-3	1.82	2.3E-3	1.89
960	1.3E-3	1.95	6.0E-4	1.95

Table 5.1: Uniform grids (NIC)

Let us now consider the second case of non-uniform smooth meshes. As mentioned earlier, these meshes can be obtained by applying some smooth transformation to uniform meshes. In this case, we consider the exponential transformation as $x = \exp(\xi)$, where ξ is the variable for which we have the uniform mesh. Such a mesh is also known as a geometric mesh. The computational domain in this case is set as $[1e - 6, 1000]$ which corresponds to the ξ domain $[\ln(1e - 6), \ln(1000)]$. It is important to note that any small positive real number can be chosen as the minimum value of x. The numerical results have been summarized in Table 5.2. Once again the numerical results show that the fixed pivot technique gives second order convergence on non-uniform smooth meshes.

	(a) $K(x, y) = k_0(x + y)$		(b) $K(x, y) = k_0xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0456	-	0.0374	-
240	0.0118	1.95	9.6E-3	1.96
480	3.0E-3	1.97	2.4E-3	2.00
960	7.6E-4	1.98	6.0E-4	2.00

Table 5.2: Non-uniform smooth grids (NIC)

The third test case has been performed on a locally uniform mesh using the same computational domain as is in the previous case. In this case we started the computation on 30 geometric mesh points, and then each cell was divided into two equal parts in the further refined levels of computation. In this way we obtained a locally uniform mesh. The EOC has been summarized in Table 5.3. Table 5.3 clearly shows that the fixed pivot technique is only first order accurate.

	(a) $K(x,y) = k_0(x+y)$		(b) $K(x,y) = k_0xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0416	-	0.0254	-
240	0.0212	0.97	0.0126	1.01
480	0.0105	1.01	6.0E-3	1.07
960	5.1E-3	1.04	2.8E-3	1.09

Table 5.3: Locally uniform grids (NIC)

Now we consider the fourth case of an oscillatory mesh to evaluate the EOC. Let us take an example of oscillatory mesh, i.e.

$$\Delta x_{i+1} := \begin{cases} 2\Delta x_i & \text{if } i \text{ is odd,} \\ \frac{1}{2}\Delta x_i & \text{if } i \text{ is even.} \end{cases}$$

Here the computational domain is same as for the first case. First, we divide the computational domain in 30 equidistant mesh points, and then each cell into two parts with 1 : 2 as per further refined levels of computation. The numerical results has been shown in Table 5.4. As expected, Table 5.4 exhibits that the fixed pivot technique is not convergent on oscillatory meshes.

	(a) $K(x,y) = k_0(x+y)$		(b) $K(x,y) = k_0xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0650	-	0.0347	-
240	0.0632	0.04	0.0309	0.16
480	0.0523	0.27	0.0257	0.26
960	0.0518	0.01	0.0253	0.01

Table 5.4: Oscillatory grids (NIC)

Finally we consider the fifth case of a non-uniform random mesh. The computations have been performed on the same domain as is for the second case. We started again with the 30 geometric mesh points, and then each cell was divided into two parts of random width in the further refined levels of computation. For each value of $I = 60, 120, 240, 480$, we performed five runs on different random grids and the relative L_1 errors were measured. The mean of these errors over five runs is used to calculate the EOC. The numerical results have been shown in Table 5.5. Table 5.5 shows clearly that the fixed pivot technique is not convergent.

	(a) $K(x,y) = k_0(x+y)$		(b) $K(x,y) = k_0xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0229	-	0.0112	-
240	0.0375	-0.71	9.4E-3	0.25
480	0.0406	-0.11	0.0135	-0.51
960	0.0402	0.01	0.0129	0.06

Table 5.5: Non-uniform random grids (NIC)

Next, we take an exponentially decreasing initial condition (EIC), namely

$$n(0,x) = \exp(-\alpha x).$$

The sum and product aggregation kernels in (5.65) are again considered. Since the analytical solution is known for the above initial conditions and kernels and can be found in [82, 2], then the experimental order of convergence can be determined by the formula

$$\text{EOC} = \ln(E_I/E_{2I})/\ln(2), \tag{5.67}$$

where E_I and E_{2I} are the L_1 error norms. The subscripts I and $2I$ correspond to the degrees of freedom. We can calculate the error E_I on a mesh with I cells. The relative error has been calculated by dividing the error $\|\mathbf{N} - \hat{\mathbf{N}}\|$ by $\|\mathbf{N}\|$. The parameter $\alpha = 10$ is taken in the above initial condition. In this case, we will again evaluate the EOC on five different type of meshes as before.

In case of uniform mesh, we set the computational domain as [0,30] to evaluate the EOC numerically. The numerical results are summarized in Table 5.6. Again, we obtain the convergence of second order numerically.

	(a) $K(x,y) = k_0(x+y)$		(b) $K(x,y) = k_0xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0486	-	0.0274	-
120	0.0135	1.84	7.2E-3	1.92
240	3.5E-3	1.94	1.9E-3	1.92
480	9.0E-4	1.96	4.8E-4	1.98

Table 5.6: Uniform grids (EIC)

Let us now evaluate the EOC on geometric grids which is a particular case of non-smooth grids. The numerical computations have been performed on the same computational domain as is for the case of geometric grids considered with the normal initial condition. The numerical results are presented in Table 5.7 which shows once again the convergence of second order.

(a) $K(x, y) = k_0(x + y)$

Grid Points	Relative Error L_1	**EOC**
60	7.1E-3	-
120	1.8E-3	1.97
240	4.5E-4	2.00
480	1.1E-4	2.03

(b) $K(x, y) = k_0xy$

Relative Error L_1	**EOC**
6.3E-3	-
1.6E-3	1.98
4.0E-4	2.00
1.0E-4	2.00

Table 5.7: Non-uniform smooth grids (EIC)

In case of availability of analytical solutions, the EOC has been computed once more on locally uniform, oscillatory and random meshes. The computational domain for locally uniform and random meshes is identical as for the previous case. However, we perform the computations on an oscillatory mesh using the same domain as is for the uniform mesh. The numerical result are demonstrated in Tables 5.8, 5.9 and 5.10. These tables show that we acquire the convergence of first order on locally uniform mesh while the fixed pivot technique is zero order convergent on oscillatory and random meshes.

(a) $K(x, y) = k_0(x + y)$

Grid Points	Relative Error L_1	**EOC**
60	0.0303	-
120	0.0156	0.96
240	7.7E-3	1.02
480	3.8E-3	1.03

(b) $K(x, y) = k_0xy$

Relative Error L_1	**EOC**
0.0145	-
7.1E-3	1.04
3.3E-3	1.08
1.6E-3	1.06

Table 5.8: Locally uniform grids (EIC)

(a) $K(x, y) = k_0(x + y)$

Grid Points	Relative Error L_1	**EOC**
60	0.0554	-
120	0.0532	0.05
240	0.0539	-0.01
480	0.0524	0.04

(b) $K(x, y) = k_0xy$

Relative Error L_1	**EOC**
0.0295	-
0.0298	-0.01
0.0279	0.09
0.0256	0.12

Table 5.9: Oscillatory grids (EIC)

	(a) $K(x,y) = k_0(x+y)$		(b) $K(x,y) = k_0 xy$	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0246	-	0.0162	-
120	0.0292	-0.25	0.0204	-0.34
240	0.0319	-0.13	0.0222	-0.12
480	0.0380	-0.25	0.0232	-0.07

Table 5.10: Non-uniform random grids (EIC)

Chapter 6

Convergence of the cell average technique for coagulation equation

In this chapter, we investigate the numerical order of convergence of the cell average technique given by J. Kumar et al. [48] to solve the non-linear pure coagulation (aggregation) equations. The convergence analysis of the scheme for these non-linear equations is still an open problem. Here we evaluate the experimental order of convergence by performing several numerical simulations and compare the numerical results obtained with those of the fixed pivot technique [38]. Similar to the previous chapter, which considered the fixed pivot technique, the main emphasis here is to evaluate experimentally the order of convergence for five different types of uniform and non-uniform meshes. The numerical experiments show that the cell average technique is second order convergent on uniform, non-uniform smooth and locally uniform meshes while the scheme is only first order accurate on oscillatory and random meshes. In spite of this, the cell average technique gives one order higher accuracy than the fixed pivot technique for locally uniform, oscillatory and random meshes.

The plan of this chapter is as follows. A brief introduction is given in the following section. The mathematical formulation of the cell average technique is reviewed in Section 6.2. In Section 6.3, we compute the experimental order of convergence of the scheme by taking few numerical examples and repeat the numerical results of the fixed pivot technique from previous chapter for the comparison.

6.1 Introduction

The nonlinear continuous coagulation equation can be solved analytically for only a few specific examples of kernels. These limitations urge us to develop new numerical techniques and study their mathematical analysis. Among all numerical sectional methods for solving these equations, the fixed pivot technique [54] is the most widely used method [13, 47]. Recently J. Kumar et al. [48] have introduced the cell average technique which preserves all advantages of the existing sectional methods. In Chapter 5, convergence analysis of the fixed pivot technique has been discussed for solving nonlinear pure coagulation equation. It has been observed that the fixed pivot technique yields second order convergence on uniform and non-uniform smooth meshes. Moreover, the scheme shows first order convergence on a locally uniform mesh. Finally the scheme is analyzed on oscillatory and random meshes, and it has been found out that unfortunately the fixed pivot technique does not converge.

The purpose of this work is to compute the experimental order of convergence of the cell average technique and to compare numerical results with the results of the fixed pivot technique discussed in the previous chapter. A brief description of the sectional methods will be directly taken from Chapter 5. In the case of uniform grids, it is easy to show the convergence analysis of the scheme for aggregation problem since both of the schemes have the same discretized formulation. In the following section, we will review the mathematical formulation of the cell average scheme for aggregation problems.

6.2 The cell average technique

The truncated version of pure coagulation equation is given as

$$\frac{\partial n(t,x)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)n(t,x-y)n(t,y)dy - \int_0^{x_{\max}} K(x,y)n(t,x)n(t,y)dy, \quad (6.1)$$

with initial condition

$$n(x,0) = n^{\text{in}}(x) \geq 0, \quad x \in \Omega :=]0, x_{\max}].$$

This technique approximates the total number of particles in finite number of cells. First of all, the continuous interval $\Omega :=]0, x_{\max}]$ is divided into a small number of cells defining size classes

$$\Lambda_i :=]x_{i-1/2}, x_{i+1/2}],\ i = 1, \ldots, I,$$

with

$$x_{1/2} = 0, \quad x_{I+1/2} = x_{\max}.$$

The representative of each size class, usually the center point of each cell $x_i = (x_{i-1/2} + x_{i+1/2})/2$, is called pivot or grid point. We introduce $\Delta x_{\min}$ and Δx to satisfy

$$\Delta x_{\min} \leq \Delta x_i = x_{i+1/2} - x_{i-1/2} \leq \Delta x.$$

For the purpose of analysis we assume quasi uniformity of the grids, i.e.

$$\frac{\Delta x}{\Delta x_{\min}} \leq C \quad (6.2)$$

where C is a positive constant. The total number of particles in the ith cell is given as

$$N_i(t) = \int_{x_{i-1/2}}^{x_{i+1/2}} n(t,x)dx.$$

Integrating the continuous equation (6.1) over the ith cell we obtain

$$\frac{dN_i}{dt} = B_i - D_i, \quad i = 1, \dots, I,$$

The total birth rate B_i and death rate D_i are given as

$$B_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx. \tag{6.3}$$

and

$$D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} K(x,y)n(t,y)n(t,x)dydx. \tag{6.4}$$

The total discrete birth and death rates of particles are evaluated by substituting the number density approximation

$$n(t,x) \approx \sum_{i=1}^{I} N_i(t)\delta(x-x_i)$$

into equations (6.12) and (6.13) as

$$\hat{B}_i = \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) K(x_k, x_j) N_j N_k, \tag{6.5}$$

and

$$\hat{D}_i = N_i \sum_{j=1}^{I} K(x_i, x_j) N_j. \tag{6.6}$$

Here $\hat{B}_i$ and $\hat{D}_i$ denote the discrete birth and death rates, respectively in the ith cell. The total volume flux V_i into cell i as a result of aggregation is given by

$$V_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x xK(x-y,y)n(t,x-y)n(t,y)dydx. \tag{6.7}$$

Similarly to the discrete birth rate the discrete volume flux can be obtained as

$$\hat{V}_i = \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) K(x_k, x_j) N_j N_k (x_j + x_k). \tag{6.8}$$

Consequently, the average volume $\overline{v}_i \in [x_{i-1/2}, x_{i+1/2}]$ of all new born particles in the ith cell can be evaluated as

$$\overline{v}_i = \frac{\hat{V}_i}{\hat{B}_i}, \quad \hat{B}_i > 0. \tag{6.9}$$

We do not need volume average $\overline{v}_i$ in case of $\hat{B}_i = 0$. However, for $\hat{B}_i = 0$ we can set $\overline{v}_i = x_i$. Here we consider that all new born particles in the ith cell are assigned temporarily at the average volume $\hat{v}_i$. If the average volume $\hat{v}_i$ is same as the pivot size x_i then the total birth $\hat{B}_i$ of new born particles can be assigned to the pivot x_i only. But this is rarely possible and hence the total particle birth $\hat{B}_i$ has to be assigned to the neighboring pivots in such a way that the total number and mass remain conserved during this reassignment. Finally, the resultant set of ODEs takes the following form

$$\frac{d\hat{N}_i}{dt} = \hat{B}_i^{CA} - \hat{D}_i^{CA}. \tag{6.10}$$

Let us consider the Heaviside function

$$H(x) := \begin{cases} 1 & \text{if } x > 0, \\ \frac{1}{2} & \text{if } x = 0, \\ 0 & \text{if } x < 0. \end{cases}$$

and

$$\lambda_i^{\pm}(x) = \frac{x - x_{i\pm 1}}{x_i - x_{i\pm 1}}. \tag{6.11}$$

Then the birth and death terms are given as

$$\begin{aligned} \hat{B}_i^{CA} =& \hat{B}_{i-1}\lambda_i^-(\overline{v}_{i-1})H(\overline{v}_{i-1} - x_{i-1}) + \hat{B}_i\lambda_i^+(\overline{v}_i)H(\overline{v}_i - x_i) \\ &+ \hat{B}_i\lambda_i^-(\overline{v}_i)H(x_i - \overline{v}_i) + \hat{B}_{i+1}\lambda_i^+(\overline{v}_{i+1})H(x_{i+1} - \overline{v}_{i+1}) \end{aligned} \tag{6.12}$$

and

$$\hat{D}_i = N_i \sum_{j=1}^{I} K(x_i, x_j) N_j. \tag{6.13}$$

The first and the fourth terms on the right hand side of equation (6.12) can be set to zero for $i = 1$ and $i = I$ respectively. The numerical approximation of $N_i(t)$ is defined by $\hat{N}_i(t)$. For the simplicity, we suppress the notation of parameter t for the rest of this chapter and use N_i instead of $N_i(t)$. The set of equations (6.10) is a discrete formulation for solving a general aggregation problem. The form of coagulation kernel and type of grids can be chosen arbitrarily. The set of equations (6.10) together with an initial condition can be solved with any higher order ODE solver to obtain number of particles in a cell $\hat{N}_i$. An appropriate solver to solve these equations is recommended in Chapter 5. The detailed formulation can be found in [48, 50].

By using (6.5) and (6.6) the cell average technique (6.10) can be written as

$$\frac{d\hat{N}_i}{dt} = \lambda_i^-(\overline{v}_{i-1})H(\overline{v}_{i-1} - x_{i-1}) \sum_{x_{i-3/2} \le x_j + x_k < x_{i-1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) K(x_k, x_j) N_j N_k$$

$$+ [\lambda_i^+(\overline{v}_i)H(\overline{v}_i - x_i) + \lambda_i^-(\overline{v}_i)H(x_i - \overline{v}_i)]$$

$$\times \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) K(x_k, x_j) N_j N_k$$

$$+ \lambda_i^+(\overline{v}_{i+1})H(x_{i+1} - \overline{v}_{i+1}) \sum_{x_{i+1/2} \le x_j + x_k < x_{i+3/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) K(x_k, x_j) N_j N_k$$

$$- N_i \sum_{j=1}^{I} K(x_i, x_j) N_j. \tag{6.14}$$

6.3 Order of convergence

In this section we take a few numerical examples where we evaluate the experimental order of convergence (EOC) on five different types of meshes. Here we consider the same test cases as are in Chapter 5. Some of numerical results of convergence from previous chapter are restated to see the difference between the two techniques. All computational details of the test cases can be found in Chapter 5. Here we discuss only numerical results for the test cases presented in the preceding chapter.

First, we consider the test case of a uniform mesh. The numerical results are presented in Tables 6.1 and 6.2. Both of the techniques show the convergence of second order. In case of uniform mesh, the cell average and the fixed pivot techniques are same for aggregation problems. Suppose analytical solutions are not available in this case. We can see from Tables 6.1 and 6.2 that the relative errors for both the schemes in numerical results are alike.

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0598	-	0.0598	-
240	0.0178	1.75	0.0178	1.75
480	5.0E-3	1.82	5.0E-3	1.82
960	1.3E-3	1.95	1.3E-3	1.95

Table 6.1: Uniform grids and $K(x, y) = k_0(x + y)$

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0306	-	0.0306	-
240	8.4E-3	1.86	8.4E-3	1.86
480	2.3E-3	1.89	2.3E-3	1.89
960	6.0E-4	1.95	6.0E-4	1.95

Table 6.2: Uniform grids and $K(x, y) = k_0xy$

Now we consider the second test case of non-uniform smooth meshes. Suppose the analytical solution is available in this case. The numerical results for the EOC have been summarized in Tables 6.3 and 6.4. Again, both the techniques clearly converge to second order.

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	6.4E-3	-	6.1E-3	-
120	1.6E-3	1.98	1.7E-3	1.86
240	4.0E-4	1.98	5.0E-4	1.88
480	1.0E-4	1.99	1.0E-4	1.87

Table 6.3: Non-uniform smooth grids and $K(x, y) = k_0(x + y)$

Let us now consider the third case of a locally uniform mesh. Here we study the same problem as is in previous case. The EOC for both the techniques has been shown in Tables 6.5 and 6.6. Once again the tables clearly show that the cell average technique is of second order while the fixed pivot technique is only first order accurate.

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	6.3E-3	-	5.7E-3	-
120	1.6E-3	1.98	1.5E-3	1.93
240	4.0E-4	2.00	3.9E-4	1.94
480	1.0E-4	2.00	1.0E-4	1.96

Table 6.4: Non-uniform smooth grids and $K(x, y) = k_0xy$

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0303	-	0.025	-
120	0.0156	0.96	8.8E-3	1.51
240	7.7E-3	1.02	2.1E-3	2.08
480	3.8E-3	1.03	5.0E-4	2.15

Table 6.5: Locally uniform grids and $K(x, y) = k_0(x + y)$

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0145	-	0.0122	-
120	7.1E-3	1.04	3.6E-3	1.75
240	3.3E-3	1.08	9.0E-4	2.01
480	1.6E-3	1.06	2.0E-4	2.17

Table 6.6: Locally uniform grids and $K(x, y) = k_0xy$

The fourth case has been performed on an oscillatory mesh. In this case, we deal with the same problem as is in first case. The numerical results have been summarized in Tables 6.7 and 6.8. Tables show that the cell average technique is first order convergent while the fixed pivot technique is not convergent.

	(a) Fixed pivot technique		(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0650	-	0.0575	-
240	0.0632	0.04	0.0273	1.07
480	0.0523	0.27	0.0131	1.06
960	0.0518	0.01	6.2E-3	1.07

Table 6.7: Oscillatory grids and $K(x, y) = k_0(x + y)$

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0347	-	0.0247	-
240	0.0309	0.16	0.0105	1.22
480	0.0257	0.26	4.8E-3	1.15
960	0.0253	0.01	2.2E-3	1.13

Table 6.8: Oscillatory grids and $K(x,y) = k_0xy$

At the end, we study the fifth case of random grids and take the same problem as are in second and third cases. The numerical results of convergence have been given in Tables 6.9 and 6.10. Once more, we obtain the first order of convergence as is in case of oscillatory grids. However, the fixed pivot technique is not convergent on oscillatory and random meshes.

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0246	-	0.0127	-
120	0.0292	-0.25	8.3E-3	0.61
240	0.0319	-0.13	4.2E-3	0.99
480	0.0380	-0.25	2.6E-3	0.70

Table 6.9: Non-uniform random grids and $K(x,y) = k_0(x+y)$

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0162	-	0.0151	-
120	0.0204	-0.34	6.0E-3	1.33
240	0.0222	-0.12	3.4E-3	0.82
480	0.0232	-0.07	2.0E-3	0.75

Table 6.10: Non-uniform random grids and $K(x,y) = k_0xy$

Chapter 7

Conclusions

In this thesis, we studied the following different issues for the continuous coagulation-fragmentation equations. Let us try to make some conclusions to each of the issue.

First, the existence of weak solutions to the continuous coagulation equation with multiple fragmentation is discussed for a large class of kernels. In particular, we extracted a weakly convergent subsequence in L^1 from a sequence of unique solutions for truncated problems by using the Dunford-Pettis-Theorem. Then it was proved that the limit function obtained from weakly convergent subsequence was actually a solution of the original continuous coagulation and multiple fragmentation equation. The uniqueness of the weak solutions was also established under more stringent assumptions on the coagulation and fragmentation kernels.

Second, the uniqueness of mass conserving solutions to the continuous coagulation and binary fragmentation equation was demonstrated with some additional restrictions on the fragmentation kernels. Here the existence of at least one mass conserving solution was due to Escobedo et al. [27] for a large class of coagulation kernels with strong binary fragmentation. More precisely, we first investigated the integrability of higher moments of the number density distribution. Then the mass conservation and application of Gronwall's lemma helped us to get the uniqueness of mass conserving solutions.

Third, we established a new existence result for the continuous coagulation and multiple fragmentation equation. The result was more general than the existence result published in Giri et al. [40]. This includes some interesting multiple fragmentation kernels which were not covered by the previous result. The existence of solutions is proven under much less restrictive conditions on the fragmentation kernels. However, the conditions on the coagulation kernels were same as before.

Next, a detailed study on the convergence analysis of the fixed pivot technique was given for solving pure coagulation equation. To show the convergence of the scheme, we studied that the scheme was consistent. The birth and death terms satisfied a Lipschitz condition. It was ascertained that the order of convergence depends on the type of the meshes chosen for the computation. The technique was second order convergent on uniform and non-uniform smooth meshes. However, it was only first order convergent on locally uniform meshes numerically. At last, the scheme was examined closely on oscillatory and non-uniform random meshes and it was observed that the technique was not convergent. Furthermore, all observations were also validated numerically. But the case of locally uniform mesh was not discussed mathematically.

Finally, we evaluated the order of convergence of the cell average technique for the pure coagulation equation by taking a few numerical examples. All numerical examples were taken from Chapter 5. The numerical results were compared with those for the case of the fixed pivot technique. It was noticed that the cell average technique was second order convergent on uniform, non-uniform smooth and locally uniform meshes. However, it gave only a first order convergence on oscillatory and random meshes. It should be pointed out that the fixed pivot technique was only first order convergent on locally uniform mesh and zero order convergent on oscillatory and random meshes. Therefore, the cell average technique enhanced the results of the convergence on non-uniform meshes.

Next, we would also like to propose some open questions for the future developments which are as follows.

- It would be interesting to know how one can enlarge the classes of kernels considered in Chapter 3 for the uniqueness of solutions to the continuous coagulation and multiple fragmentation equation.

- It is not easy to extend the classes of kernels where we proved the existence of solutions for coagulation equation with multiple fragmentation. According to our knowledge, the present approach is not sufficient for the extension. We think that, to extend the classes of coagulation kernels in such a way that the case of singular coagulation kernels can be covered, one has to restrict the initial data. This gives us more restrictions on the space.

- The existence of equilibrium solutions and asymptotic properties for time-dependent solutions for the continuous coagulation and binary fragmentation equation are discussed in [22, 92]. Asymptotic behaviour of solutions to the discrete coagulation-fragmentation equation is also examined in [10, 11]. These issues should also be covered for the continuous coagulation equation with multiple fragmentation.

- To show the existence and uniqueness for two-dimensional coagulation-fragmentation equations in both the discrete and the continuous case.

- The possible occurrence of instantaneous gelation in discrete coagulation equation is discussed in [12, 96]. This should also be demonstrated for the continuous coagulation equation.

- Here we did not discuss the mathematical convergence analysis of the cell average technique for solving pure coagulation equation. However, the scheme enhances the numerical order of convergence on locally uniform, oscillatory and random meshes. It would be fascinating to explain how we can obtain the same orders of convergence by means of mathematical analysis.

Appendix A

Inequalities

To compare the classes of kernels in the study of continuous coagulation-fragmentation equation, we need the following inequalities.

Proposition A.0.1. *For any x, $y > 0$, the following inequalities hold*

$$2^{p-1}(x^p + y^p) \leq (x+y)^p \leq x^p + y^p \quad \textit{if} \;\; 0 \leq p \leq 1, \tag{A.1}$$

$$2^{p-1}(x^p + y^p) \geq (x+y)^p \geq x^p + y^p \quad \textit{if} \;\; p \geq 1, \tag{A.2}$$

and

$$2^{p-1}(x^p + y^p) \geq (x+y)^p \quad \textit{if} \;\; p < 0. \tag{A.3}$$

Proof. For a given $x > 0$, we set

$$f(y) = (x+y)^p - (x^p + y^p).$$

We can see that $f(0) = 0$. By taking the derivative with respect to y, we obtain

$$f'(y) = p[(x+y)^{p-1} - y^{p-1}].$$

This implies that $f'(y) \leq 0$ if $p \leq 1$ and $f'(y) \geq 0$ if $p \geq 1$ i.e. $f(y)$ is monotonically decreasing if $p \leq 1$ and monotonically increasing if $p \geq 1$. Thus, we have

$$(x+y)^p \leq x^p + y^p \;\; \text{if} \;\; 0 \leq p \leq 1, \text{and} \;\; (x+y)^p \geq x^p + y^p \;\; \text{if} \;\; p \geq 1.$$

For $p = 1$, the first inequality of (A.2) is obvious. Assume $p > 1$ for that case. For a given $x > 0$, we set

$$g(y) = 2^{p-1}(x^p + y^p) - (x+y)^p.$$

Now taking the derivative with respect to y, we obtain

$$g'(y) = p[(2y)^{p-1} - (x+y)^{p-1}].$$

To determine the critical point, we take

$$g'(y) = p[(2y)^{p-1} - (x+y)^{p-1}] = 0$$

which gives us $y = x$ as the only critical point. Again taking the derivative with respect to y, we get

$$g''(y) = p(p-1)[2^{p-1}y^{p-2} - (x+y)^{p-2}].$$

So, we obtain

$$[g''(y)]_{y=x} = p(p-1)2^{p-2}x^{p-2} > 0 \text{ if } p > 1 \text{ and } p < 0$$

$$< 0 \text{ if } 0 < p < 1.$$

Therefore we have a minimum at $y = x$ if $p > 1$ and $p < 0$. For $0 < p < 1$ we have a maximum at $y = x$. Now we find

$$g(x) = 2^{p-1}(2x^p) - (2x)^p = 0.$$

Thus, we have

$$g(y) \geq 0 \text{ if } p > 1 \text{ and } p < 0$$

i.e.

$$2^{p-1}(x^p + y^p) \geq (x+y)^p \text{ if } p \geq 1 \text{ and } p < 0$$

holds in (A.2) and (A.3). For the first inequality of (A.1) we see that

$$g(y) \leq 0 \text{ if } 0 < p < 1$$

giving

$$2^{p-1}(x^p + y^p) \leq (x+y)^p \text{ if } 0 \leq p \leq 1.$$

□

Proposition A.0.2. *For any x, $y > 0$, the following inequalities hold*

$$x^p y^p \leq x^p + y^p \quad \text{if } 0 < x \leq 1 \text{ or } 0 < y \leq 1 \text{ for any } p \geq 0, \tag{A.4}$$

$$2x^p y^p \geq x^p + y^p \quad \text{if } x, y \geq 1 \text{ and } p \geq 0, \tag{A.5}$$

$$2x^p y^p \leq x^p + y^p \quad \text{if } x, y \geq 1 \text{ and } p < 0, \tag{A.6}$$

$$2(1+x)^p(1+y)^p \geq (1+x)^p + (1+y)^p \quad \text{if } x, y > 0 \text{ and } p \geq 0, \tag{A.7}$$

and

$$2(1+x)^p(1+y)^p \leq (1+x)^p + (1+y)^p \quad \text{if } x, y > 0 \text{ and } p < 0. \tag{A.8}$$

Proof. For a given $x > 0$, we set

$$f(y) = x^p y^p - (x^p + y^p).$$

We can see that $f(0) = -x^p$ and $f(1) = -1$. Now taking the derivative with respect to y, we obtain

$$f'(y) = py^{p-1}[x^p - 1].$$

This implies that $f'(y) \leq 0$ for $p \geq 0$ if $x \leq 1$. Thus, $f(y)$ is monotonically decreasing for $p \geq 0$ if $x \leq 1$. Therefore, the proof of (A.4) is complete. For the inequalities (A.5) and (A.6), we have

$$2x^p y^p = x^p y^p + x^p y^p \geq x^p + y^p \quad \text{if} \quad x, y \geq 1 \quad \text{and} \quad p \geq 0,$$

$$\leq x^p + y^p \quad \text{if} \quad x, y \geq 1 \quad \text{and} \quad p < 0.$$

But the inequalities (A.7) and (A.8) can be directly obtained by (A.5) and (A.6) respectively. ☐

Proposition A.0.3. *For any x, $y > 0$ and any α, β, $p \in \mathbb{R}$, the following inequalities hold*

$$(1+x)^\alpha (1+y)^\beta + (1+x)^\beta (1+y)^\alpha \leq 2(1+x)^p (1+y)^p \quad \textit{where} \quad p \geq \max\{\alpha, \beta\},$$

$$(1+x)^\alpha (1+y)^\beta + (1+x)^\beta (1+y)^\alpha \geq 2(1+x)^p (1+y)^p \quad \textit{where} \quad p \leq \min\{\alpha, \beta\}.$$

Proposition A.0.4. *For any x, $y > 0$, the following results are true*

$$(1+x+y)^p \leq (1+x)^p + (1+y)^p \leq 2(1+x)^p(1+y)^p \quad \textit{if} \quad 0 < p \leq 1, \tag{A.9}$$

$$(1+x+y)^p \leq 2^{p-1}[(1+x)^p + (1+y)^p] \leq 2^p(1+x)^p(1+y)^p \quad \textit{if} \quad p \geq 1, \tag{A.10}$$

$$2(1+x+y)^p \leq (1+x)^p + (1+y)^p \quad \textit{if} \quad p < 0, \tag{A.11}$$

$$(1+x)^p + (1+y)^p \leq 2^p(1+x+y)^p \quad \textit{if} \quad p \geq 1. \tag{A.12}$$

Proof. The inequalities in (A.9) and (A.10) can be easily proved by using the second inequality of (A.1) and the first inequality of (A.2) respectively with (A.7). For (A.11), we find that

$$\frac{(1+x)^p + (1+y)^p}{(1+x+y)^p} = \frac{(1+x)^p}{(1+x+y)^p} + \frac{(1+y)^p}{(1+x+y)^p} \geq 1 + 1 = 2 \quad \text{if} \quad p < 0.$$

Finally for (A.12), we have

$$(1+x+y)^p = \frac{1}{2^p}(2+2x+2y)^p \geq \frac{1}{2^p}(2+x+y)^p \geq \frac{1}{2^p}[(1+x)^p + (1+y)^p] \quad \text{if} \quad p \geq 1.$$

☐

Proposition A.0.5. *For any x, $y > 0$, take α, $\beta \in \mathbb{R}$ with $\alpha \cdot \beta \geq 0$ and set $\lambda = \alpha + \beta$. Then we obtain the estimates*

$$x^\alpha y^\beta + x^\beta y^\alpha \leq x^\lambda + y^\lambda, \tag{A.13}$$

and

$$(1+x)^\alpha (1+y)^\beta + (1+x)^\beta (1+y)^\alpha \leq (1+x)^\lambda + (1+y)^\lambda. \tag{A.14}$$

Proof. For $\alpha = 0$ or $\beta = 0$ both inequalities (A.13) and (A.14) hold. Assume that $\alpha \cdot \beta > 0$. We know that Young's inequality holds, i.e.

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q} \quad \text{where} \quad \frac{1}{p} + \frac{1}{q} = 1 \quad \text{with} \quad p, q \in]1, \infty[\quad \text{and} \quad a, b \geq 0.$$

Substituting $a = x^\alpha$ and $b = y^\beta$ in the above inequality, we find that

$$x^\alpha y^\beta \leq \frac{x^{\alpha p}}{p} + \frac{y^{\beta q}}{q}.$$

Choose $p = \frac{\alpha+\beta}{\alpha}$ and $q = \frac{\alpha+\beta}{\beta}$ then $\frac{1}{p} + \frac{1}{q} = 1$. This implies for $\lambda = \alpha + \beta$

$$x^\alpha y^\beta \leq \frac{\alpha}{\lambda} x^\lambda + \frac{\beta}{\lambda} y^\lambda. \tag{A.15}$$

Interchanging x and y in (A.15), we obtain

$$y^\alpha x^\beta \leq \frac{\alpha}{\lambda} y^\lambda + \frac{\beta}{\lambda} x^\lambda. \tag{A.16}$$

By adding (A.15) and (A.16), we obtain

$$x^\alpha y^\beta + x^\beta y^\alpha \leq x^\lambda + y^\lambda.$$

The above inequality gives us

$$(1+x)^\alpha (1+y)^\beta + (1+x)^\beta (1+y)^\alpha \leq (1+x)^\lambda + (1+y)^\lambda.$$

□

Proposition A.0.6. *For any $\lambda \in [0, 1[$, $x > 0$ and $y' \in]0, x[$, there exists a constant $k_\lambda(y') > 0$ such that*

$$y^\lambda + (x-y)^\lambda - x^\lambda \geq k_\lambda(y') y^\lambda \quad \textit{for any} \quad y \in]0, y'[.$$

Note that $k_\lambda(y') \to 0$ for $y' \to x$.

Proof. Let us suppose that

$$f(y) = y^{-\lambda}[x^{\lambda} - (x-y)^{\lambda}].$$

Then

$$f'(y) = -\lambda y^{-(\lambda+1)} x[x^{\lambda-1} - (x-y)^{\lambda-1}].$$

This implies that

$$f'(y) \geq 0 \;\text{ for any }\; 0 < y < x.$$

Now choose $c \in]0,1[$ such that $y \leq cx = y'$, then

$$f(y) \leq f(cx)$$

i.e.

$$y^{-\lambda}[x^{\lambda} - (x-y)^{\lambda}] = f(y) \leq f(cx) = c^{-\lambda}x^{-\lambda}[x^{\lambda} - (x-cx)^{\lambda}]$$

$$= c^{-\lambda}[1-(1-c)^{\lambda}].$$

Multiplying by y^{λ} on both side, we get

$$x^{\lambda} - (x-y)^{\lambda} \leq c^{-\lambda}[1-(1-c)^{\lambda}]y^{\lambda} + y^{\lambda} - y^{\lambda}.$$

We set $k_{\lambda}(y') = 1 - c^{-\lambda}[1-(1-c)^{\lambda}]$ and obtain

$$y^{\lambda} + (x-y)^{\lambda} - x^{\lambda} \geq k_{\lambda}(y')y^{\lambda}.$$

The limit $y' \to x$ corresponds to $c \to 1$. By using the second inequality of (A.1), it can be easily shown that $k_{\lambda}(y') > 0$. □

Appendix B

Kernels and their classes

This chapter is divided into four different sections. A list of a few specific coagulation kernels from the literature is given in Section B.1. Sections B.2 and B.3 contain the classes of coagulation kernels that were considered in conjuction with respectively binary and multiple fragmentation by various authors. In Section B.4, we make an overview of various classes of coagulation kernels and their relations to each other. Finally, some bounds on non-singular coagulation kernels from Subsection B.1.1 are given in Section B.5.

B.1 Coagulation kernels

In this section, we provide a list of coagulation kernels which are of substantial interest in many areas of application. Let us divide them into the following two types.

B.1.1 Nonsingular coagulation kernels

In the following kernels $k > 0$ is a suitable constant.

Smoluchowski (1917) [87]: *Shear kernel (linear velocity profile)*, see also [2, 86, 64]

$$K(x, y) = k(x^{1/3} + y^{1/3})^3. \tag{B.1}$$

Schumann (1940) [81]: *Gravitational kernel*, see also [2, 86]

$$K(x, y) = k(x^{1/3} + y^{1/3})^2|x^{2/3} - y^{2/3}|. \tag{B.2}$$

Stockmayer (1943) [93]: *Polymerisation kernel*, see also [2, 86]

$$K(x, y) = k(x + c)(y + c). \tag{B.3}$$

Shiloh et al. (1973) [84]: *Shear kernel (non-linear velocity profile)*, see also [2, 86]

$$K(x, y) = k(x^{1/3} + y^{1/3})^{7/3}. \tag{B.4}$$

Ding et al. (2006) [16]: *Activated sludge flocculation*

$$K(x,y) = k\frac{(x^{1/3}+y^{1/3})^q}{1+\left(\frac{x^{1/3}+y^{1/3}}{2y_c^{1/3}}\right)^3} \quad \text{where} \quad 0 \le q < 3. \tag{B.5}$$

Here q is the order of the kernel.

Koch et al. (2007) [46]: *Modified Smoluchowski kernel*

$$K(x,y) = k\frac{(x^{1/3}+y^{1/3})^2}{x^{1/3}\cdot y^{1/3}+c}. \tag{B.6}$$

B.1.2 Singular at the origin or on the axes

Smoluchowski (1917) [87]: *Brownian diffusion kernel*, see also [2, 86]

$$\begin{aligned} K(x,y) &= k(x^{1/3}+y^{1/3})(x^{-1/3}+y^{-1/3}) \\ &= k\frac{(x^{1/3}+y^{1/3})^2}{x^{1/3}\cdot y^{1/3}}. \end{aligned} \tag{B.7}$$

Kapur (1972) [45]: *Granulation kernel*

$$K(x,y) = k\frac{(x+y)^a}{(x\cdot y)^b}. \tag{B.8}$$

Sastry (1975) [80]: *Non-random coalescence kernel*

$$K(x,y) = k(x^{2/3}+y^{2/3})\left(\frac{1}{x}+\frac{1}{y}\right). \tag{B.9}$$

Hounslow (1998) [43]: *Equi-partition of kinetic energy (EKE) kernel (Granulation)*, see also [95]

$$K(x,y) = k(x^{1/3}+y^{1/3})^2\sqrt{\frac{1}{x}+\frac{1}{y}}. \tag{B.10}$$

Peglow (2005) [73]: *A granulation kernel*

$$K(x,y) = k\frac{(x+y)^{0.7105}}{(x\cdot y)^{0.0621}}. \tag{B.11}$$

B.2 Classes of coagulation kernels considered in conjunction with binary fragmentation kernels

This section presents a few classes of coagulation kernels which were used to prove the existence of solutions for the continuous coagulation and binary fragmentation equation. A coagulation kernel belongs to such a class if there exists a suitable constant k such that an estimate of the type defining the class holds for all $x,\ y \geq 0$. The following classes were considered in the literature:

Stewart (1990) [89]

$$K(x,y) \leq k[(1+x)^\alpha + (1+y)^\alpha] \text{ for some } 0 \leq \alpha < 1 \text{ and positive constant } k. \tag{B.12}$$

Dubovskiǐ (1996) [21]

$$K(x,y) \leq k(1+x+y), \quad k > 0. \tag{B.13}$$

Dubovskiǐ (2001) [19]

$$K(x,y) \leq k(1+x)(1+y), \quad k > 0. \tag{B.14}$$

Laurençot (2002) [60]

$$K(x,y) \leq k(1+x)(1+y), \quad k > 0 \tag{B.15}$$

with the following growth condition. For each $R \in \mathbb{R}_{>0}$, there holds

$$\lim_{y\to\infty} \sup_{x\in]0,R[} \frac{K(x,y)}{y} = 0.$$

Escobedo et al. (2003) [27]

$$K(x,y) \leq k(1+x+y)^\lambda, \quad \text{with } \lambda \in [0,2] \text{ and } k > 0,$$

and

$$K(x,y) \leq k[(1+x)^\alpha(1+y)^\beta + (1+x)^\beta(1+y)^\alpha], \quad \text{with } 0 \leq \alpha \leq \beta \leq 1 \text{ and } k > 0. \tag{B.16}$$

B.3 Classes of coagulation kernels considered in conjunction with multiple fragmentation kernels

In this section, we provide a few classes of coagulation kernels which were considered in the literature to show the existence of solutions to the continuous coagulation and multiple fragmentation equation. A coagulation kernel belongs to such a class if there exists a suitable constant k such that an estimate of the type defining the class holds for all x, $y \geq 0$. These classes are as follows:

McLaughlin et al. (1997) [66]

$$K(x,y) \text{ is constant.} \tag{B.17}$$

Melzak(1957) [70] and Lamb (2004) [56]

$$K(x,y) \text{ is bounded.} \tag{B.18}$$

Laurençot (2000) [57]

$$K(x,y) = r(x)r(y) + \alpha(x,y), \tag{B.19}$$

where r and α are non-negative functions satisfying

$$\begin{cases} r \in \mathcal{C}(\mathbb{R}_{\geq 0}; \mathbb{R}_{\geq 0}), \quad \alpha \in \mathcal{C}({\mathbb{R}^2}_{\geq 0}; \mathbb{R}_{\geq 0}), \\ \\ 0 \leq \alpha(x,y) = \alpha(y,x) \leq Ar(x)r(y), \qquad (x,y) \in [1,\infty[^2, \end{cases}$$

for some positive real number A.

Escobedo et al. (2005) [29]

$$K(x,y) = x^\alpha y^\beta + x^\beta y^\alpha, \quad \text{with} \quad -1 \leq \alpha \leq 0 \leq \beta \leq 1. \tag{B.20}$$

Giri et al. (2010) [40]

$$K(x,y) \leq k(1+x)^\alpha (1+y)^\alpha, \quad \text{for some} \quad 0 \leq \alpha < 1 \quad \text{and} \quad k > 0. \tag{B.21}$$

B.4 Summary of classes

For any x, $y > 0$, and p, α, $\beta \in \mathbb{R}$ and for some arbitrary constants $k > 0$ we consider the following classes using various growth functions $w(x,y)$.

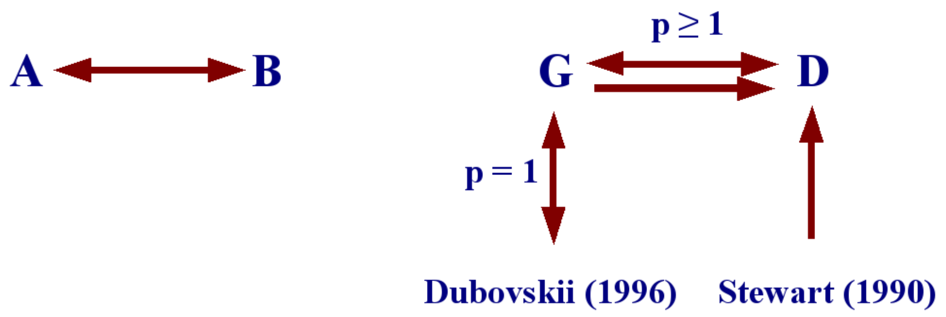
A : $w(x,y) = k(x^p + y^p)$, **B** : $w(x,y) = k(x+y)^p$,
C : $w(x,y) = kx^p y^p$, **D** : $w(x,y) = k[(1+x)^p + (1+y)^p]$,
E : $w(x,y) = k(1+x)^p(1+y)^p$, **F** : $w(x,y) = k[(1+x)^\alpha(1+y)^\beta + (1+x)^\beta(1+y)^\alpha]$,
G : $w(x,y) = k(1+x+y)^p$, **H** : $w(x,y) = k[x^\alpha y^\beta + x^\beta y^\alpha]$.

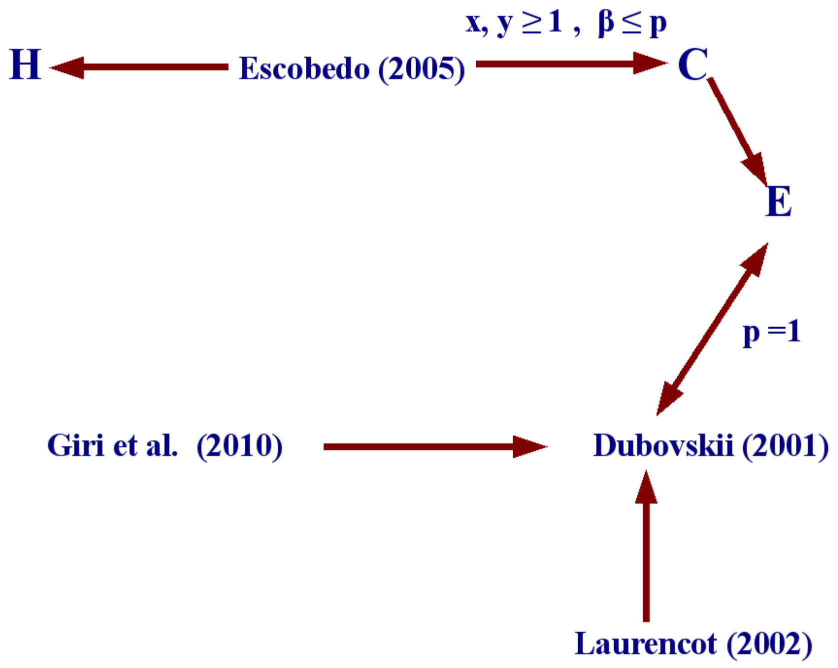
The constant k must be finite but may be arbitrarly large. A coagulation kernel $K(x,y)$ belongs to a class $A,\ldots,H$ if it is estimated by the growth function defining the class as follows

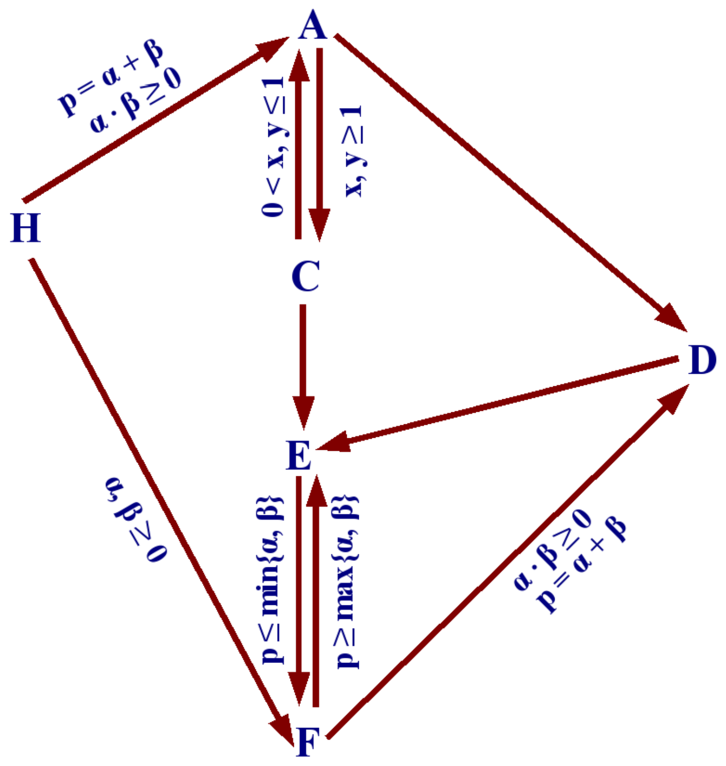
$$K(x,y) \leq w(x,y) \quad \text{for all} \quad x,y \geq 0.$$

Now we will compare these classes by drawing the following pictures where $\mathbf{X} \longrightarrow \mathbf{Y}$ or $\mathbf{X} \longleftrightarrow \mathbf{Y}$ imply that $\mathbf{X}$ is contained in $\mathbf{Y}$ or both are equivalent, respectively.

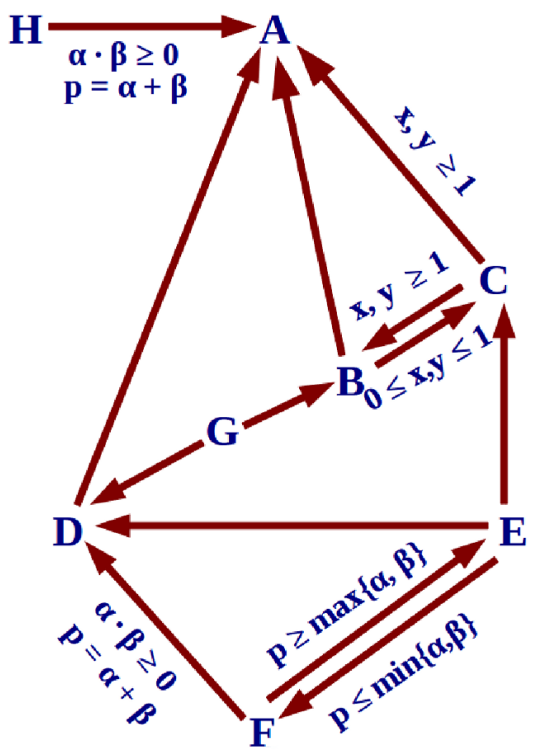
Case I $\quad p \geq 0$






A
H
C
D
E
F
p= α + β
α · β ≥ 0
0 < x, y ≤ 1
x, y ≥ 1
α, β ≥ 0
p ≤ min{α, β}
p ≥ max{α, β}
α · β ≥ 0
p = α + β

Case II $p < 0$


H
A
α · β ≥ 0
p = α + β
x, y ≥ 1
C
x, y ≥ 1
B
0 ≤ x,y ≤ 1
G
D
E
α · β ≥ 0
p = α + β
p ≥ max{α, β}
p ≤ min{α,β}
F

B.5 Bounds on non-singular kernels

This section shows the bounds for class **E** on the non-singular coagulation kernels which were listed in Subsection B.1.1. These bounds are obtained as follows by using (A.7) from Proposition A.0.2. We distinguish the case $p \geq 1$ and $\alpha \in [0, 1[$.

(B.1) Shear kernel (linear velocity profile)

$$\begin{aligned} K(x, y) &= k(x^{1/3} + y^{1/3})^3 \\ &\leq k[(1+x)^{1/3} + (1+y)^{1/3}]^3 \leq 2^3 k(1+x)(1+y) \\ &\leq k_1(1+x)^p(1+y)^p \quad \text{for} \quad p = 1. \end{aligned}$$

This kernel lies in the class (B.14) considered by Dubovskii (2001).

(B.2) Gravitational kernel

$$\begin{aligned} K(x, y) &= k(x^{1/3} + y^{1/3})^2 |x^{2/3} - y^{2/3}| \\ &\leq k[(1+x)^{1/3} + (1+y)^{1/3}]^2 [(1+x)^{2/3} + (1+y)^{2/3}] \\ &\leq 2^2 k(1+x)^{2/3}(1+y)^{2/3} \cdot 2(1+x)^{2/3}(1+y)^{2/3} \leq k_1(1+x)^{4/3}(1+y)^{4/3} \\ &\leq k_1(1+x)^p(1+y)^p \quad \text{where} \quad p = \frac{4}{3}. \end{aligned}$$

This kernel lies in the class **E** for $p = \frac{4}{3}$.

(B.4) Shear kernel (non-linear velocity profile)

$$\begin{aligned} K(x, y) &= k(x^{1/3} + y^{1/3})^{7/3} \\ &\leq k[(1+x)^{1/3} + (1+y)^{1/3}]^{7/3} \leq 2^{7/3} k(1+x)^{7/9}(1+y)^{7/9} \\ &\leq k_1(1+x)^\alpha(1+y)^\alpha \quad \text{where} \quad \alpha = \frac{7}{9} \in [0, 1[. \end{aligned}$$

This kernel lies in the class (B.21) considered by Giri et al. (2010).

(B.5) Ding et al. (activated sludge flocculation)

$$\begin{aligned} K(x, y) &= k \frac{(x^{1/3} + y^{1/3})^q}{1 + \left(\frac{x^{1/3} + y^{1/3}}{2y_c^{1/3}}\right)^3} \quad \text{where} \quad 0 \leq q < 3 \\ &\leq k(x^{1/3} + y^{1/3})^q \\ &\leq k[(1+x)^{1/3} + (1+y)^{1/3}]^q \leq 2^q k(1+x)^{q/3}(1+y)^{q/3} \\ &\leq k_1(1+x)^\alpha(1+y)^\alpha \quad \text{where} \quad \alpha = \frac{q}{3} \in [0, 1[. \end{aligned}$$

This kernel lies in the class (B.21) considered by Giri et al. (2010).

(B.6) Modified Smoluchowski kernel

$$\begin{aligned}
K(x,y) &= k\frac{(x^{1/3}+y^{1/3})^2}{x^{1/3}\cdot y^{1/3}+c} \quad \text{where} \quad c>0 \\
&\leq \frac{k}{c}(x^{1/3}+y^{1/3})^2 \\
&\leq \frac{k}{c}[(1+x)^{1/3}+(1+y)^{1/3}]^2 \leq 2^2\frac{k}{c}(1+x)^{2/3}(1+y)^{2/3} \\
&\leq k_1(1+x)^{\alpha}(1+y)^{\alpha} \quad \text{where} \quad \alpha=\frac{2}{3}\in [0,1[.
\end{aligned}$$

This kernel lies in the class (B.21) considered by Giri et al. (2010).

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