MASTER

Mean field limit for general interacting particle systems

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Abstract

In the report, we investigate interacting particle systems. An interacting particle system is a stochastic system which describes the behaviour of a large number of discrete objects, the particles. The behaviour of a particle depends on the configuration of the other particles in the system. By construction of the generator, we formulate the forward Kolmogorov equation describing the stochastic evolution of this system. Existence and uniqueness of a solution for a truncated version of this forward Kolmogorov equation are investigated and the existence of a solution to the original system is proven. Thereafter, we consider the interacting particles on a discrete grid, scale the grid size and let this grid size go to zero. This limit is called the mean field limit and leads to a deterministic system of integro-differential equations. We consider an application of interacting particles in terms of a tumor growth model and investigate this particle system and the mean field limit by means of simulations.

Chapter 1

Introduction

In the last decade, much research has been conducted on interacting particle systems. Interacting particle systems consist of a large number of discrete objects, the particles, whose behaviour depends on the distribution of the other particles in the system. Interacting particles can be used to model biological phenomena such as ecological systems [5], crowd dynamics [6] and disease models [8]. In literature, we find examples of multi-component interacting particle systems, for example in [3], [4]. In these models, different types of particles occur which enable the investigation of the dynamics in systems where the types of the particles are relevant to the behaviour of the entire system.

From the microscopic description of a system of interacting particles, the macroscopic behaviour can be determined by establishing the mean-field limit [3], [5], [8]. The mean field limit is the limit taken after appropriate scaling of the system. There are several ways to scale the system. For example, in [3] the intensities of the interactions in the system are scaled. Furthermore, they accelerate birth and investigate the limiting behaviour. In [5], the interacting particle system is formulated on the space $\mathbb{R}^d$ and the limiting behaviour is investigated by letting the number of particles converge to infinity. Moreover, in [8], the mean field limit is established for a specific example on $\mathbb{Z}$. The limit can provide a deterministic description in the form of ODEs, PDEs or integro-differential equations. On the other hand, the microscopic description through interacting particles is stochastic.

In this report, we want to investigate interacting particle systems in a general setting. Similar to [3], [4], we consider a multiple types interacting particle system. Furthermore, we consider a generally formulated generator that describes birth of particles, transitions from one type of particle to another and the death of particles. This generator depends on the rate functions which encode the rates of birth, transition or death of a particle. The generator is used to formulate the forward Kolmogorov equation describing the evolution of the probability distribution.

To formulate the forward Kolmogorov equation, we find the adjoint operator of the generator of the interacting particle system. Constructing the adjoint explicitly enables us to prove statements about the well-posedness of this evolution equation. The construction of the adjoint uses a change of variables formula applicable to the different parts of the generator.

We investigate the well-posedness of the evolution equation. By assuming certain regularities and boundedness of the rate functions, existence and uniqueness of solutions can be verified in the general setting for a truncated version of the forward Kolmogorov equation. We extend the existence result to the original forward Kolmogorov equation by applying the Ascoli-Arzelà's theorem.

Next, we determine the mean field limit for the interacting particle system. We make some additional assumptions on the rates and the configuration space. Nonetheless, we formulate the interacting particle system in a general way. Then we scale the system and take the limit which leads to a system of integro-differential equations.

The motivation behind the determination of the mean field limit is that the analysis of the macroscopic model is easier than for the microscopic model. Simulation of the solution in the macroscopic model is faster than the simulation for the microscopic model. The investigation of the microscopic model is also useful, however, since we can use biological theory to describe the microscopic behaviour and to determine the transition rates. Mean field theory provides the link between the microscopic and the macroscopic model.

We apply the obtained results to a tumor growth model. This tumor growth model is based on the model from [7]. In this paper, tumor growth is modelled by including layers of different cell types: proliferative cells, non-proliferative cells and necrotic cells. Informally, proliferative cells are living tumor cells that can divide, non-proliferative cells are living tumor cells that cannot divide and necrotic cells are dead tumor cells that still occupy volume. In this paper, they consider a fixed ratio between the radius of the tumor and the thickness of the different layers.

In our report, we formulate a different tumor growth model based on the ideas of [7]. We describe tumor growth as an interacting particle system and use the biological background in [7] to determine an expression for the rate functions. We use the mean field limit to investigate tumor growth and simulate both the solution to the system of integro-differential equations as well as the interacting particle system for different grid sizes.

First, we consider a two-dimensional tumor growth model. We simulate the solution of the derived mean field limit, the original interacting particle system and some scaled versions of this particle system. However, in the investigation of the limiting behaviour, we encounter systems that are too large to solve. Therefore, we also consider a one-dimensional interacting acting particle system. In this lower-dimensional system, we can accurately investigate the limiting behaviour.

We shortly describe the structure of this report. In Chapter 2, we formulate the mathematical framework behind interacting particle systems. A general interacting particle system is defined and we formulate the generator for this system. Furthermore, we introduce the reference measure $\hat{\Pi}^k$ which is also used in the literature on multiple particle systems, see for example [4]. Lastly, we introduce the forward Kolmogorov equation, describing the evolution of this system.

In Chapter 3, we formulate a general change of variables formula. The first section of this chapter is meant to provide us with a useful tool, given by Lemma 3.1.1, used in several other proofs throughout the report. Moreover, in this Chapter the formula is used to determine the general adjoint operator for the generator of an interacting particle system under certain assumptions on the rate functions. This adjoint operator is given in Lemma 3.2.1.

In Chapter 4, the first step towards the well-posedness of our evolution equation is made. We consider a truncated version of the forward Kolmogorov equation. In this version, the rate functions are truncated, leading to a sequence of solutions for the truncated system. The result of well-posedness for this truncated system is formalized in Theorem 4.1.4.

Chapter 5 contains useful a priori estimates such as a first and second moment bound. Both bounds are used to prove existence of a solution to the forward Kolmogorov equation. Moreover, this chapter provides a derivation of an entropy estimate. These estimates can be viewed as a summary of the necessary stepping stones needed to mathematically prove the extension of the well-posedness results found in Chapter 4. We consider weak solutions and apply Ascoli-Arzelà's theorem to ensure the existence of a convergent subsequence of our sequence of solutions. Moreover, we prove the convergence in the weak problem.

Chapter 6 describes the mean field limit for a generally formulated interacting particle system. We consider a compact set in a $\mathbb{Z}^d$ grid and scale this grid size. Then we take the limit to find a system of integro-differential equations. Finally, we prove the well-posedness of this system.

Chapter 7 contains a detailed explanation of an application of this theory by consideration of a tumor growth model. We formulate this model as a specific interacting particle system with four different cell types. The rate functions satisfy the assumption made in the general setting which means we can use the well-posedness results we found there. Furthermore, we can investigate the mean field limit found in Chapter 6. To verify the results, we simulate the solution of the integro-differential equation, the original interacting particle system and two scaled versions of the interacting particles system. We plot the radius of the tumor against the density of the cell types and plot the number of particles at each time. Since we investigate scaling, we want to decrease our grid size. For our ODE solution, we want to consider the finest grid. However, this leads to more demanding computations, resulting in a problem that is too large to solve. Therefore, we also consider an example of a one-dimensional tumor growth model in this chapter. If we assume spherical symmetry, this model can be regarded as the diameter of the tumor. In this one-dimensional case, we clearly see the convergence of the scaled interacting particle systems to the ODE solution.

Chapter 2

Model description

In this chapter, we introduce mathematical concepts considered throughout this project. Firstly, we explain the definition of an interacting particle system. We introduce the Markov generator that describes the dynamics of the interacting particle system. Next, we define the Lebesgue-Poisson measure. This all provides us with a framework to define an evolution equation describing the distribution of this system. This evolution equation is called the forward Kolmogorov equation.

2.1 Interacting particles system

In this report, we consider a general multiple types interacting particle system. An interacting particle system is a model which describes the interaction of a large amount of discrete objects, the particles. In this report, we investigate a general interacting particle model where k different types of particles exist. These particles form a configuration on a compact set X and this configuration evolves over time. We assume the process behaves as a continuous-time Markov process. Three types of changes can occur in this configuration: new particles of each type can be born into the system, particles can transition from one type to another and particles of each type can die all with exponential rates. The precise value of these rates at a specific time depends on the configuration at that time solely.

To explain the notion of an interacting particle system better, we consider an example. [9] describes the spread of the corona virus by modeling it as an interacting particle system. Individuals have one of three possible types: susceptible, infected or recovered/died. Susceptible people can get infected. Their rate of transition depends on the types of the people surrounding them. When a susceptible individual is surrounded by many infected people the rate of transition is high. Likewise, when no infected people are near, the rate of transition is zero. Once an individual is infected, it will either recover or die after some time. This rate of transition is constant and does not depend on the configuration. Individuals that are in the state recovered/died remain in this state. This model is an example of an interacting particle system with three different types of particles. No births into the system occur, but the model could be extended to consider births as well. This disease model shows one possible way the configuration changes the rates of transitions. In accordance with our intuition, the likelihood of a susceptible person getting infected becomes larger when this person is surrounded by individuals that are infected themselves. The Markov property is also clear in this example, since the rates of transition only depend on the current transition and are independent of previous configurations.

2.2 Finite point measures

As mentioned before, the configuration of particles in this model follows a continuous time Markov process where the rates of birth, death and transition at time t depend solely on the configuration at time t. Therefore, we want to introduce notation to describe the configuration of particles. We want to describe these configurations as finite point measures. A set of finite point measures is denoted by $\mathcal{M}(X)$. Since we want to distinguish k different types of particles and we assume that each particle can only have one type at most, we can describe the location of particles as a vector of the form $(\nu_1, ..., \nu_k) = (\sum_{i_1=1}^{n_1} \delta_{x_{i_1}}, \ldots, \sum_{i_k=1}^{n_k} \delta_{x_{i_k}}) \in \hat{\Gamma}_X$, where

$$\hat{\Gamma}_X := \{(\nu_1, \ldots, \nu_k) \in [\mathcal{M}(X)]^k : \text{supp } \nu_i \cap \text{supp } \nu_j = \emptyset \quad \forall i, j \in \{1, \ldots, k\}, i \neq j\}.$$

In this report, we sometimes use a slight abuse of notation, saying $x \in \nu_i$, for $i \in \{1, \ldots, k\}$, where we mean $x \in \text{supp } \nu_i$. This is done to shorten notation.

We want to consider the total variation norm on measures ν. This norm is defined as

Definition 2.2.1. Let $\nu \in \hat{\Gamma}_X$, then the total variation norm is defined as

$$\|\nu\|_{TV} := \sup_{g \in C_0(X^k), \|g\|_\infty \leq 1} \langle g, \nu \rangle,$$

where $\langle \cdot, \cdot \rangle$ denotes the duality product.

2.3 Generator

The evolution of this system can be described by the generator. In the formulation of the generator, we consider the types of changes that can occur and the rates of these different types of changes. The first one is birth of particles. Let for all $m \in \{1, \ldots, k\}, e_m$ denote the unit normal vector. Then we say a particle of type m is born at position $y \in X$ when the following change occurs

$$\nu \mapsto \nu + \delta_y e_m \qquad \text{for } y \notin \text{supp } \nu.$$

The second possible change is the transition of a particle from one type to another. We denote the transition of a particle y from type i to type j as

$$\nu \mapsto \nu - \delta_y e_i + \delta_y e_j \qquad \text{for } y \in \text{supp } \nu_i.$$

Thirdly, we consider the death of particles. The death of a particle of type l at position $y \in X$ is denoted as

$$\nu \mapsto \nu - \delta_y e_l \qquad \text{for } y \in \text{supp } \nu_l.$$

We want to consider a generator that tackles all these possible changes. One of the reasons, we aim to construct this generator is that it enables us to formulate an evolution equation solved by a probability distribution describing this stochastic process. The definition of a Markov generator relies on the definition of the Markov pregenerator, which is given in [10] as

Definition 2.3.1. A linear operator L on $C(X)$ with domain $\mathcal{D}(L)$ is said to be a Markov pregenerator if it satisfies the following conditions:

1. $\mathbf{1} \in \mathcal{D}(L)$ and $L\mathbf{1} = 0$.
2. $\mathcal{D}(L)$ is dense in $C(X)$.
3. If $f \in \mathcal{D}(L)$, $\alpha \geq 0$, and $f - \alpha L f = g$, then

$$\min_{\zeta \in X} f(\zeta) \geq \min_{\zeta \in X} g(\zeta).$$

The definition of the Markov generator is then according to [10] given by

Definition 2.3.2. A Markov generator is a closed Markov pregenerator L which satisfies

$$\mathcal{R}(I - \alpha L) = C(X) \tag{2.3.1}$$

for all sufficiently small positive α.

These definitions are technical, but [10] also explains that we can construct the generator if we know the possible changes that can occur and the rates that belong to these changes. Based on [4], we can informally say the generator has the form

$$L = L_\beta + L_\tau + L_\delta,$$

where L_β can be seen a generator corresponding to birth in the system, L_τ as a generator corresponding to the transitions of a particle from one type to another and L_δ as a generator corresponding deaths within the system. The generator operates on an observable function F.

Definition 2.3.3. For $F \in L^\infty(\hat{\Gamma}_X, \hat{\Pi}^k)$, the generator of an interacting particle system is given by

$$LF(\nu) = L_\beta F(\nu) + L_\tau F(\nu) + L_\delta F(\nu), \tag{2.3.2}$$

where

$$L_\beta F(\nu) := \sum_{m=1}^{k} \int_X [F(\nu + \delta_y e_m) - F(\nu)]\kappa_{0m}(y, \nu)\lambda(dy), \tag{2.3.3}$$

$$L_\tau F(\nu) := \sum_{i=1, j\neq i}^{k} \sum_{x \in \nu_i} [F(\nu - \delta_x e_i + \delta_x e_j) - F(\nu)]\kappa_{ij}(x, \nu), \tag{2.3.4}$$

$$L_\delta F(\nu) := \sum_{l=1}^{k} \sum_{x \in \nu_l} [F(\nu - \delta_y e_l) - F(\nu)]\kappa_{l0}(x, \nu). \tag{2.3.5}$$

Here κ_{ij} are the rate functions for all $i, j \in \{0, \dots, k\}, i \neq j$.

In the first part of this generator we integrate over X because this part corresponds to a birth in the system and this can happen at every unoccupied $x \in X$. In the other two parts of the generator, we consider sums rather than integrals because we sum over existing particle.

Throughout this report, we make the following assumptions on the rates.

Assumption 2.3.4.

(i) $\kappa_{ij}(x, \cdot) \in L^\infty(\hat{\Gamma}_X, \hat{\Pi}^k)$ for all $i, j \in \{0, \dots, k\}, i \neq j$, i.e. for all $i, j \in \{1, \dots, k\}, i \neq j$, there exists a constant $\overline{\kappa_{ij}}$ such that $\kappa_{ij}(x, \nu) \leq \overline{\kappa_{ij}}$ for all $x \in X, \nu \in \hat{\Gamma}_X$.

(ii) $\kappa_{0m}(y, \underline{\omega}) = 0$ if $y \in \text{supp } \underline{\omega}$ for all $m \in \{1, \dots, k\}$.

(iii) $\kappa_{ij}(y, \omega) = 0$ if $y \notin \text{supp } \omega_i$ for all $i, j \in \{1, \dots, k\}, i \neq j$.

(iv) $\kappa_{l0}(y, \omega) = 0$ if $y \notin \text{supp } \omega_l$.

(v) There exists a constant C_β such that $\int_X \kappa_{0m}(y, \nu)\lambda(dy) \leq C_\beta \|\nu\|_{TV} \overline{\kappa_{0m}}$ for all $m \in \{1, \dots, k\}$.

(vi) There exists a constant C_δ such that $\int_X \kappa_{l0}(y, \nu)\lambda(dy) \leq C_\delta \|\nu\|_{TV} \overline{\kappa_{l0}}$ for all $l \in \{1, \dots, k\}$.

Note that Assumption 2.3.4 (i) includes both births, transitions and deaths. In the remainder of this report, we consider a uniform bound for all rate functions. We say

$$\overline{\kappa} := \max\{\overline{\kappa_{ij}} | i, j \in \{0, \dots, k\}, i \neq j\}.$$

Furthermore, intuitively, Assumption 2.3.4 (ii) says that a particle cannot be born at position $y \in X$ if there is already another particle at that position. Similarly, Assumption 2.3.4 (iii) says a particle cannot transition from type i to type j if it is not type i to begin with and according to Assumption 2.3.4 (iv) a particle of type l cannot die at position $y \in X$, if the particle is not of type l to begin with.

2.4 Lebesgue-Poisson measure

We want to equip the space $\hat{\Gamma}_X$ with measure $\hat{\Pi}^k$. To handle the disjoint union of particles, we first define a measure Π^k on the set $\Gamma_X = [\mathcal{M}(X)]^k$. We note that $\hat{\Gamma}_X \subset \Gamma_X$.

The idea behind the measure we are going to construct is that we want to sum over each possible configuration and count the number of particles in each configuration, where the type of particle is irrelevant in this count.

Firstly, we consider a system with only one type of particles, i.e. $k = 1$. Then we define [4]

$$\Lambda^n : \bigsqcup_{n=0}^{\infty} X^n \to [\mathcal{M}(X)] \quad \text{as the mapping} \quad (x_1^1, ..., x_m^1) \mapsto \sum_{i=1}^{m} \delta_{x_i^1}.$$

The next step is to define a measure over this set $\bigsqcup_{n=0}^{\infty} X^n$. This measure is called the Lebesgue-Poisson measure.

First of all, if we consider $B = (x_1^1, \dots, x_m^1) \subset \bigsqcup_{n=0}^{\infty} X^n$, then we say $\lambda(B) := |B| = \#B = m$.

What we want, is to define a measure λ^∞ on the whole set $\bigsqcup_{n=0}^{\infty} X^n$. Hence, we want to count the number of particles in each possible subset of $\bigsqcup_{n=0}^{\infty} X^n$. The ordering of the points in this set is irrelevant. This intensity measure λ^∞ is defined as

$$\lambda^\infty := \sum_{n=0}^{\infty} \frac{1}{n!} \lambda^{\otimes n}. \tag{2.4.1}$$

We divide here by $n!$ because we can order particles $(x_1^1, \dots, x_n^1)$ in $n!$ different ways. Since the ordering is irrelevant when we want to count the number of particles, we divide by the number of options. Furthermore, since this measure, λ^∞, is defined on the domain of Λ^n and the range of Λ^n is the set of finite measures $\mathcal{M}(X)$, we can define the reference measure Π on the set $\mathcal{M}(X)$ as a push-forward $\Pi := \Lambda^n_{\#} \lambda^\infty$.

This means for $k = 1$, we have for a measurable function $f(\nu) \in L^1(\hat{\Gamma}_X, \Pi)$ that

$$\int_{\hat{\Gamma}_X} f(\nu) d\Pi := \sum_{n=0}^{\infty} \frac{1}{n!} \int_{X^n} f \circ \Lambda^n d\lambda^{\otimes n}.$$

In an interacting particle system with multiple types, we define the mapping

$$\Lambda^{n,k} : \left[\bigsqcup_{n=0}^{\infty} X^n \right]^k \to [\mathcal{M}(X)]^k \quad \text{as} \quad \left((x_1^1, \dots, x_{n_1}^1), \dots, (x_1^k, \dots, x_{n_k}^k)\right) \mapsto \left(\sum_{i=1}^{n_1} \delta_{x_i^1}, \dots, \sum_{i=1}^{n_k} \delta_{x_i^k} \right). \tag{2.4.2}$$

We define measure Π^k on a set $[\mathcal{M}(X)]^k$ as $\Pi^k := \otimes^k \Pi$. Hence, for a function $f(\nu) \in L^1(\Gamma_X, \Pi^k)$, we have

$$\int_{\Gamma_X} f(\nu) d\Pi^k(\nu) := \sum_{n_1,\dots,n_k=0}^{\infty} \frac{1}{\prod_{p=1}^{k} n_p!} \int_{X^{n_1}} \cdots \int_{X^{n_k}} f \circ \Lambda^{n,k} d\lambda^{\otimes n_1} \dots d\lambda^{\otimes n_k}.$$

To summarize, we constructed a measure Π^k on the set Γ_X. However, we describe all the possible configurations by $\hat{\Gamma}_X \subset \Gamma_X$. Hence, we want to formulate a measure that is zero when there exists ν_i and ν_j that are not disjoint for some $i, j \in \{1, \dots, k\}, i \neq j$. This is accomplished by defining the measure $\hat{\Pi}^k$ as follows

Definition 2.4.1.

$$\hat{\Pi}^k(\nu) := \begin{cases} \Pi^k(\nu) & \text{if } \nu \in \hat{\Gamma}_X, \\ 0 & \text{otherwise.} \end{cases} \tag{2.4.3}$$

In other words, this construction means that for some function $f(\nu) \in L^1(\hat{\Gamma}_X, \hat{\Pi}^k)$, we have

$$\int_{\hat{\Gamma}_X} f(\nu) d\hat{\Pi}^k(\nu) := \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{1}{\prod_{p=1}^k n_p!} \int_{X^{n_1}} \cdots \int_{X^{n_k}} \mathbb{1}_{\hat{\Gamma}_X} \circ \Lambda^{n,k} f \circ \Lambda^{n,k} d\lambda^{\otimes n_1} \ldots d\lambda^{\otimes n_k}.$$

Lemma 2.4.2. Let measure $\hat{\Pi}^k$ be given by (2.4.3) and let X be a compact set, such that $\lambda(X) < \infty$, then it holds that

$$\int_{\hat{\Gamma}_X} d\hat{\Pi}^k(\nu) < \infty.$$

Proof. By definition, we have

$$\begin{aligned} \int_{\hat{\Gamma}_X} d\hat{\Pi}^k(\nu) &= \sum_{n_1,\ldots,n_k} \frac{1}{\prod_{p=1}^k n_p!} \int_{X^{n_1}} \cdots \int_{X^{n_k}} \mathbb{1}_{\hat{\Gamma}_X} \circ \Lambda^{n,k} d\lambda^{\otimes n_1} \ldots d\lambda^{\otimes n_k}, \\ &\leq \sum_{n_1,\ldots,n_k} \prod_{p=1}^{k} \frac{\lambda(X)^{n_p}}{n_p!} = e^{k\lambda(X)}. \end{aligned}$$

□

Since we want to ensure the finiteness of measure $\hat{\Pi}^k$, we assume throughout this report that $\lambda(X) < \infty$.

2.5 Forward Kolmogorov equation

We study the time evolution of the distribution of the interacting particle system. From [4], we know that these distributions satisfy the following evolution equation if they exist

$$\frac{d}{dt}\langle F, \rho_t \rangle = \langle LF, \rho_t \rangle, \quad \forall F \in L^\infty(\hat{\Gamma}_X, \hat{\Pi}^k), \tag{2.5.1}$$

with initial condition

$$\rho_t \Big|_{t=0} = \rho_0 \tag{2.5.2}$$

Here $\langle \cdot, \cdot \rangle$ denotes the duality product. The operator L is the generator of this system given by (2.3.2).

Since equation (2.5.1) has to hold for all $F \in L^\infty(\hat{\Gamma}_X, \hat{\Pi}^k)$, we say that if ρ_t is a solution to (2.5.1) then it is a solution to the forward Kolmogorov equation

$$\frac{d}{dt}\rho_t = L^* \rho_t, \tag{2.5.3}$$

where L^* is the adjoint of L.

We want to establish well-posedness of this system. Therefore, we start by determining the exact form of the adjoint operator. To do this, we first want to formulate an auxiliary lemma describing a change of variables formula with respect to the measure $\hat{\Pi}^k$. This happens in the next chapter.

Chapter 3

Forward Kolmogorov equation

3.1 Change of variables formula

We want to determine the exact form of the forward Kolmogorov equation. Therefore, we first introduce an auxiliary lemma in this section. This lemma provides a change of variables formula which will be used throughout this report and helps us determining the exact form of the forward Kolmogorov equation.

Lemma 3.1.1. Let $g_{0m}(y,\underline{\omega}) : X \times \hat{\Gamma}_X \to \mathbb{R}_0^+, m \in \{1,\dots,k\}$ be functions such that $g_{0m}(y,\underline{\omega}) = 0$ if $y \in \text{supp } \underline{\omega}$ and $g_{0m}(y,\cdot) \in L^1(\hat{\Gamma}_X, \Pi^k)$. Furthermore, for $i,j \in \{1,\dots,k\}$ with $i \neq j$, let $g_{ij}(x,\underline{\omega}) : X \times \hat{\Gamma}_X \to \mathbb{R}_0^+$ be functions such that $g_{ij}(x,\underline{\omega}) = 0$ if $x \notin \text{supp } \omega_i$ and $g_{ij}(x,\cdot) \in L^1(\hat{\Gamma}_X, \Pi^k)$. Let $g_{l0}(y,\underline{\omega}) : X \times \hat{\Gamma}_X \to \mathbb{R}_0^+, l \in \{1,\dots,k\}$ be functions such that $g_{l0}(y,\underline{\omega}) = 0$ if $y \notin \text{supp } \nu_l$ and $g_{l0}(y,\cdot) \in L^1(\hat{\Gamma}_X, \Pi^k)$. Furthermore, let $F \in L^\infty(\hat{\Gamma}_X, \Pi^k)$. Then the following equalities hold:

$$
\begin{aligned}
&\int_{\hat{\Gamma}_X} \sum_{m=1}^{k} \int_X F(\nu + \delta_y e_m) g_{0m}(y,\nu)\lambda(dy) d\hat{\Pi}^k(\nu) = \int_{\hat{\Gamma}_X} F(\nu) \sum_{m=1}^{k} \sum_{x\in\nu_m} g_{0m}(x, \nu - \delta_x e_m) d\hat{\Pi}^k(\nu), \\
&\int_{\hat{\Gamma}_X} \sum_{i,j\neq i}^{k} \sum_{x\in\nu_i} F(\nu - \delta_x e_i + \delta_x e_j) g_{ij}(x,\nu) d\hat{\Pi}^k(\nu) = \int_{\hat{\Gamma}_X} F(\nu) \sum_{i,j\neq i}^{k} \sum_{x\in\nu_j} g_{ij}(x, \nu + \delta_x e_i - \delta_x e_j) d\hat{\Pi}^k(\nu), \\
&\int_{\hat{\Gamma}_X} \sum_{l=1}^{k} \sum_{x\in\nu_l} F(\nu - \delta_x e_l) g_{l0}(x,\nu) d\hat{\Pi}^k(\nu) = \int_{\hat{\Gamma}_X} F(\nu) \sum_{l=1}^{k} \int_X g_{l0}(y, \nu + \delta_y e_l)\lambda(dy) d\hat{\Pi}^k(\nu).
\end{aligned}
\tag{3.1.1}
$$

This lemma is formulated very generally. Note, however, that if we consider the functions g_{0m}, g_{ij} and g_{l0} to be a product of rate functions satisfying Assumption 2.3.4 and L^1-functions then the conditions in the lemma are satisfied. Intuitively, in view of the interacting particle system, the first equation corresponds to the births into the system. In this lemma, we consider the possibility that every particle can be born in the system. The second equation corresponds with transitions between state i to state j. Lastly, the third equation corresponds to cell death. The proof of this lemma can be found in Appendix A.

3.2 Forward Kolmogorov equation

Next, we want to determine the adjoint operator for the generator of a general type of interacting particle systems. Under Assumption 2.3.4, we can determine the adjoint operator with the help of Lemma 3.1.1.

Lemma 3.2.1. For a general interacting particle system with rates satisfying Assumption 2.3.4, we have the following adjoint operator

$$L^*u = L^*_\beta u + L^*_\tau u + L^*_\delta u, \tag{3.2.1}$$

where

$$L^*_\beta u := \sum_{m=1}^{k} \left(\sum_{x\in\nu_m} \kappa_{0m}(x,\nu-\delta_x e_m)u(\nu-\delta_x e_m) - \kappa_{0m}(X,\nu)u(\nu) \right), \tag{3.2.2}$$

$$L^*_\tau u := \sum_{i,j=1,i\neq j}^{k} \left(\sum_{x\in\nu_j} \kappa_{ij}(x,\nu+\delta_x e_i-\delta_x e_j)u(\nu+\delta_x e_i-\delta_x e_j) - \sum_{x\in\nu_i} \kappa_{ij}(x,\nu)u(\nu) \right), \tag{3.2.3}$$

$$L^*_\delta u := \sum_{l=1}^{k} \left(\int_X \kappa_{l0}(y,\nu+\delta_y e_l)u(\nu+\delta_y e_l) - \sum_{x\in\nu_l} \kappa_{l0}(x,\nu)u(\nu) \right). \tag{3.2.4}$$

Here, $\kappa_{0m}(X,\nu) := \int_X \kappa_{0m}(y,\nu)\lambda(dy)$ and u is the Radon-Nikodym derivative of ρ.

If $\rho(d\nu)$ is absolutely continuous with respect to the reference measure $\hat{\Pi}^k$, then $\rho(d\nu) = u(\nu)d\hat{\Pi}^k(\nu)$, where u is the Radon-Nikodym derivative.

Proof. When considering the birth part of the generator we have by the definition of the adjoint operator that

$$\langle F, L^*_\beta \rho\rangle = \langle L_\beta F, \rho\rangle.$$

Furthermore, we know

$$\langle L_\beta F, \rho\rangle = \int_{\hat{\Gamma}_X} \left(\sum_{m=1}^{k} \int_X [F(\nu+\delta_y e_m) - F(\nu)]\kappa_{0m}(y,\nu)\lambda(dy) \right) u(\nu)d\hat{\Pi}^k(\nu),$$

By application of Lemma 3.1.1, it holds that

$$= \int_{\hat{\Gamma}_X} \sum_{m=1}^{k} \left(\sum_{x\in\nu_m} \kappa_{0m}(x,\nu-\delta_x e_m)u(\nu-\delta_x e_m) - \int_X \kappa_{0m}(y,\nu)\lambda(dy)u(\nu) \right) F(\nu)d\hat{\Pi}^k(\nu).$$

From this, we can conclude that

$$L^*_\beta u = \sum_{m=1}^{k} \left(\sum_{y\in\nu_m} \kappa_{0m}(y,\nu-\delta_y e_m)u(\nu-\delta_y e_m) - \kappa_{0m}(X,\nu)u(\nu) \right).$$

□

The proofs for the transition and death part work analogously.

Chapter 4

Truncated forward Kolmogorov equation

4.1 Well-posedness in mild sense

We want to prove that the system (2.5.1) is well-posed. To do so, we first prove in this section the well-posedness of a truncated version of this system. The reason for the investigation of this truncated system is that we want to apply a well-posedness theorem for which all the requirements are met by this truncated system but not necessarily by the original system. Once well-posedness is established for this truncated system, we extend these results in Chapter 5. The truncated system is given by:

$$\begin{cases} \frac{d}{dt}u_t = L_M^* u_t, \\ u_0 = \bar{u}. \end{cases} \tag{4.1.1}$$

Here, L_M^* is defined for fixed $M \in \mathbb{N}$ as

$$L_M^* u := L_{M,\beta}^* u + L_{M,\tau}^* u + L_{M,\delta}^* u, \tag{4.1.2}$$

where

$$L_{M,\beta}^* u := \sum_{m=1}^{k} \left(\sum_{x \in \nu_m} \kappa_{0m}^M(x, \nu - \delta_x e_m) u(\nu - \delta_x e_m) - \kappa_{0m}^M(X, \nu) u(\nu) \right), \tag{4.1.3}$$

with for all $m \in \{1, \dots, k\}$

$$\kappa_{0m}^M(x, \nu) := \begin{cases} 0 & \text{if } |\nu_m| \geq M, \\ \kappa_{0m}(x, \nu) & \text{otherwise.} \end{cases} \tag{4.1.4}$$

Furthermore,

$$L_{M,\tau}^* u := \sum_{i,j \neq i}^{k} \left(\sum_{x \in \nu_j} \kappa_{ij}^M(x, \nu + \delta_x e_i - \delta_x e_j) u(\nu + \delta_x e_i - \delta_x e_j) - \sum_{x \in \nu_i} \kappa_{ij}^M(x, \nu) u(\nu) \right), \tag{4.1.5}$$

with for all $i, j \in \{1, \dots, k\}, i \neq j$

$$\kappa_{ij}^M(x, \nu) := \begin{cases} 0 & \text{if } |\nu_i| \geq M, \\ \kappa_{ij}(x, \nu) & \text{otherwise.} \end{cases} \tag{4.1.6}$$

Moreover,

$$L^*_{M,\delta}u := \sum_{l=1}^{k}\left(\int_X \kappa^M_{l0}(y,\nu+\delta_y e_l)u(\nu+\delta_y e_l)\lambda(dy) - \sum_{x\in\nu_l}\kappa^M_{l0}(x,\nu)u(\nu)\right), \tag{4.1.7}$$

with for all $l \in \{1,\dots,k\}$

$$\kappa^M_{l0}(x,\nu) := \begin{cases} 0 & \text{if } |\nu_l| \geq M, \\ \kappa_{l0}(x,\nu) & \text{otherwise.} \end{cases} \tag{4.1.8}$$

We note that for the truncated rates, it holds that

$$\|\nu\|_{TV}\,\kappa^M_{ij}(x,\nu) \leq M\overline{\kappa} \qquad \text{for all } i,j\neq i \in \{0,\dots,k\}. \tag{4.1.9}$$

To shorten notation, we define the operators $\Lambda^+_\beta, \Lambda^+_\tau$ and Λ^+_δ as follows

$$\Lambda^+_\beta u_t := \sum_{m=1}^{k}\sum_{x\in\nu_m}\kappa^M_{0m}(x,\nu-\delta_x e_m)u_t(\nu-\delta_x e_m), \tag{4.1.10}$$

$$\Lambda^+_\tau u_t := \sum_{i,j\neq i}^{k}\sum_{x\in\nu_j}\kappa^M_{ij}(x,\nu+\delta_x e_i-\delta_x e_j)u_t(\nu+\delta_x e_i-\delta_x e_j), \tag{4.1.11}$$

$$\Lambda^+_\delta u_t := \sum_{l=1}^{k}\int_X \kappa^M_{l0}(y,\nu+\delta_y e_l)u_t(\nu+\delta_y e_l)\lambda(dy). \tag{4.1.12}$$

Moreover, we say

$$\Lambda^+ u_t := \Lambda^+_\beta u_t + \Lambda^+_\tau u_t + \Lambda^+_\delta u_t.$$

Furthermore, we define

$$\gamma^-_\beta(\nu) := \sum_{m=1}^{k}\kappa^M_{0m}(X,\nu), \tag{4.1.13}$$

$$\gamma^-_\tau(\nu) := \sum_{i,j\neq i}^{k}\sum_{x\in\nu_i}\kappa^M_{ij}(x,\nu), \tag{4.1.14}$$

$$\gamma^-_\delta(\nu) := \sum_{l=1}^{k}\sum_{x\in\nu_l}\kappa^M_{l0}(x,\nu). \tag{4.1.15}$$

We say that

$$\gamma^-(\nu) := \gamma^-_\beta(\nu) + \gamma^-_\tau(\nu) + \gamma^-_\delta(\nu). \tag{4.1.16}$$

Therefore, we can write $L^*_M u_t(\nu)$ as

$$L^*_M u_t(\nu) = \Lambda^+ u_t(\nu) - \gamma^-(\nu)u_t(\nu). \tag{4.1.17}$$

Since we aim to investigate the existence and uniqueness of a solution to (4.1.1), we have to define what a solution is. However, first we give meaning to the notions of absolute continuity and differentiability.

Definition 4.1.1. Let X be a Banach space. A continuous function $u : [0,T] \to X$ is said to be

1. *absolutely continuous* if there exists a function $g \in L^1([0,T];X)$ such that

$$\|u_t - u_s\|_X \leq \int_s^t g(r)\, dr \qquad \text{for any } 0 \leq s < t \leq T.$$

We denote by $AC((0,T);X)$ the space of absolutely continuous functions from $(0,T)$ to X.

2. *differentiable* at $t \in (0,T)$ if there exists some $g \in X$, such that

$$\lim_{|h|\to 0} \left\| \frac{u_{t+h} - u_t}{h} - g \right\|_X = 0.$$

In this case, we denote the derivative of u at $t \in (0,T)$ by $u'(t) = g$.

Lemma 4.1.2. Let X be a reflexive Banach space and $u \in AC([0,T];X)$. Then there exists $g \in L^1([0,T];X)$ such that u is almost everywhere differentiable with $g(t) = u'(t)$ for almost every $t \in (0,T)$ and the fundamental theorem of calculus holds:

$$u_t = u_0 + \int_0^t g(r)\, dr \qquad \text{for every } t \in [0,T].$$

For the proof of this lemma see Proposition 3.22 of [14].

Let $W := L^1(\hat{\Gamma}_X, \hat{\Pi}^k) \cap L^\infty(\hat{\Gamma}_X, \hat{\Pi}^k)$ equipped with norm $\|\cdot\|_W := \|\cdot\|_{L^1} + \|\cdot\|_{L^\infty}$. Then we have the following definition of a solution to (4.1.1)

Definition 4.1.3. A continuous function $u : [0,T] \to W$ is said to be a *mild* solution of (4.1.1) with initial datum $\bar{u} \in W$, if

$$u_t = \bar{u} + \int_0^t L_M^* u_r\, dr \qquad \text{for all } t \in [0,T].$$

In the following, we consider the closed subset of $D \subset W$ defined by

$$D := \{u \in L^1(\hat{\Gamma}_X, \hat{\Pi}^k) \cap L^\infty(\hat{\Gamma}_X, \hat{\Pi}^k) : u(\nu) \in [0,\infty) \quad \text{for } \hat{\Pi}^k\text{-almost every } \nu \in \hat{\Gamma}_X\}. \tag{4.1.18}$$

We want to prove that under Assumption 2.3.4, system (4.1.1) with initial condition $u_0 = \bar{u} \in D$ has a unique solution in the sense of Definition 4.1.3.

Reformulation into a fixed-point problem. First of all, we formally note that if $u_t \in D$ is a solution to (4.1.1), we have that

$$\frac{d}{dt}\big(e^{\gamma^-(\nu)t} u_t(\nu)\big) = \gamma^-(\nu) e^{\gamma^-(\nu)t} u_t(\nu) + e^{\gamma^-(\nu)t} \frac{d}{dt} u_t(\nu) = e^{\gamma^-(\nu)t} \Lambda^+ u_t(\nu).$$

If we take the integrated version, this leads to

$$u_t(\nu) = u_0(\nu) e^{-\gamma^-(\nu)t} + \int_0^t e^{-\gamma^-(\nu)(t-s)} \Lambda^+ u_s(\nu)\, ds.$$

In view of the previous discussion, we define the mapping $T : C([0,T];D) \to C([0,T];D)$ as

$$(Tv)(t,\nu) := v_0(\nu) e^{-\gamma^-(\nu)t} + \int_0^t e^{-\gamma^-(\nu)(t-s)} \Lambda^+ v_s(\nu)\, ds \tag{4.1.19}$$

We claim there exists a one-to-one relation between solutions of (4.1.1) and fixed points of T. Therefore, we first prove T has a unique fixed point.

Theorem 4.1.4. *Let D be given by (4.1.18) and let T be the operator as defined in (4.1.19), where the rate functions satisfy Assumption 2.3.4. Then operator T has a unique fixed point for each $M \in \mathbb{N}$.*

Proof. We aim to use the Banach Fixed Point Theorem. We want to prove that if $v \in C([0,T];D)$, this implies $Tv \in C([0,T];D)$. We split the proof into several steps.

Step 1. Positivity

We first note that if $v \in C([0,T];D)$, then $v_t(\nu) \geq 0$ for all $t \in [0,T]$ and $\hat{\Pi}^k$-almost every $\nu \in \hat{\Gamma}_X$. Therefore,

$$(Tv)(t,\nu) \geq 0 \qquad \text{for all } t \in [0,T] \text{ and } \hat{\Pi}^k\text{-almost every } \nu \in \hat{\Gamma}_X.$$

Step 2. L^∞ bound

Applying the Assumption 2.3.4 and using bound (4.1.9), we obtain

$$\begin{aligned}
\left\|\Lambda_\beta^+ v_s\right\|_{L^\infty} &\leq kM\overline{\kappa}\left\|v_s\right\|_{L^\infty},\\
\left\|\Lambda_\tau^+ v_s\right\|_{L^\infty} &\leq \binom{k}{2}M\overline{\kappa}\left\|v_s\right\|_{L^\infty},\\
\left\|\Lambda_\delta^+ v_s\right\|_{L^\infty} &\leq kMC_\delta\overline{\kappa}\left\|v_s\right\|_{L^\infty}.
\end{aligned}$$

Therefore, if we define $C_\infty := \overline{\kappa}M(k + \binom{k}{2} + kC_\delta)$, we have that

$$\begin{aligned}
\left\|Tv(t,\cdot)\right\|_{L^\infty} &\leq \left\|v_0\right\|_{L^\infty} + \operatorname{esssup}_{\nu\in\hat{\Gamma}_X}\int_0^t \Lambda^+ v_s(\nu)\,ds,\\
&\leq \left\|v_0\right\|_{L^\infty} + tC_\infty \sup_{s\in[0,t]}\left\|v(s,\cdot)\right\|_{L^\infty} < \infty.
\end{aligned}$$

Step 3. L^1 bound

We also have to show that $Tv \in L^1(\hat{\Gamma}_X, \hat{\Pi}^k)$. Therefore, we first make estimates on $\Lambda_\beta^+, \Lambda_\tau^+$ and Λ_δ^+. We start with the birth part.

$$\begin{aligned}
\int_{\hat{\Gamma}_X} |\Lambda_\beta^+ v_s(\nu)| d\hat{\Pi}^k(\nu) &\leq \sum_{m=1}^k \int_{\hat{\Gamma}_X}\left(\sum_{x\in\nu_m}|\kappa_{0m}^M(x,\nu-\delta_x e_m)v_s(\nu-\delta_x e_m)|\right)d\hat{\Pi}^k(\nu),\\
&\overset{(*)}{=} \sum_{m=1}^k \int_{\hat{\Gamma}_X}|\kappa_{0m}^M(X,\nu)v_s(\nu)|\,d\hat{\Pi}^k(\nu),\\
&\leq kC_\beta\overline{\kappa}M\left\|v_s\right\|_{L^1} < \infty.
\end{aligned}$$

Here, $(*)$ follows from application of Lemma (3.1.1) where $F(\nu) = 1$ for all $\nu \in \hat{\Gamma}_X$.

For the transition part, we have

$$\begin{aligned}
\int_{\hat{\Gamma}_X} |\Lambda_\tau^+ v_s| d\hat{\Pi}^k &\leq \int_{\hat{\Gamma}_X}\sum_{i,j\neq i}^k\sum_{x\in\nu_j}|\kappa_{ij}^M(x,\nu+\delta_x e_i-\delta_x e_j)v_s(\nu+\delta_x e_i-\delta_x e_j)|d\hat{\Pi}^k(\nu),\\
&\overset{(**)}{=} \sum_{i\neq j}^k\int_{\hat{\Gamma}_X}\sum_{x\in\nu_i}|\kappa_{ij}^M(x,\nu)v_s(\nu)|\,d\hat{\Pi}^k(\nu),\\
&\leq \binom{k}{2}\overline{\kappa}M\left\|v_s\right\|_{L^1} < \infty.
\end{aligned}$$

Here, $(**)$ follows by application of Lemma 3.1.1 where $F(\nu) = 1$ for all $\nu \in \hat{\Gamma}_X$.

Lastly, we want to find a bound for the death part. We have

$$\int_{\hat\Gamma_X} |\Lambda^+_\delta v_s(\nu)| d\hat\Pi^k(\nu) \le \int_{\hat\Gamma_X} \sum_{l=1}^k \int_X |\kappa^M_{l0}(y,\nu+\delta_y e_l) v_s(\nu+\delta_y e_l)| \lambda(dy) d\hat\Pi^k(\nu),$$
$$\overset{(***)}{=} \int_{\hat\Gamma_X} \sum_{l=1}^k \sum_{x\in\nu_l} |\kappa^M_{l0}(x,\nu) v_s(\nu)| d\hat\Pi^k(\nu),$$
$$\le k\overline{\kappa} M \|v_s\|_{L^1} < \infty.$$

Here, $(***)$ follows again by application of Lemma 3.1.1 where $F(\nu)=1$ for all $\nu \in \hat\Gamma_X$.

If we define $C_1 := \overline{\kappa} M (C_\beta k + \binom{k}{2} + k)$, we find

$$\|Tv(t,\cdot)\|_{L^1} \le \|v_0\|_{L^1} + \int_{\hat\Gamma_X} \int_0^t \Lambda^+ v_s(\nu) ds d\hat\Pi^k,$$
$$\le \|v_0\|_{L^1} + tC_1 \sup_{s\in[0,t]} \|v(s,\cdot)\|_{L^1} < \infty.$$

Step 4. Supremum bound in time and continuity

Moreover, we want to show that $\sup_{t\in[0,T]} \|Tv(t,\cdot)\|_W < \infty$ and $t \mapsto Tv(t,\cdot)$ is continuous.

If we define $C_W := C_1 + C_\infty$, we have that

$$\sup_{t\in[0,T]} \|Tv(t,\cdot)\|_W = \sup_{t\in[0,T]} \left\| v_0 e^{-\gamma^-(\cdot)t} + \int_0^t e^{-\gamma^-(\cdot)(t-s)} \Lambda^+ u_s ds \right\|_W,$$
$$\le \sup_{t\in[0,T]} \|v_0\|_W + tC_W \sup_{s\in[0,t]} \|v(s,\cdot)\|_W,$$
$$\le \|v_0\|_W + TC_W \sup_{s\in[0,T]} \|v(s,\cdot)\|_W < \infty.$$

Furthermore, it holds that

$$\sup_{t\in[0,T]} \|Tv(t+h,\cdot) - Tv(t,\cdot)\|_W$$
$$= \sup_{t\in[0,T]} \left\| v_0 e^{-\gamma(\cdot)(t+h)} + \int_0^{t+h} e^{-\gamma^-(\cdot)(t+h-s)} \Lambda^+ v_s ds - v_0 e^{-\gamma^-(\cdot)t} - \int_0^t e^{-\gamma^-(\cdot)(t-s)} \Lambda^+ v_s ds \right\|_W,$$
$$\le \sup_{t\in[0,T]} \left(e^{-\gamma^-(\cdot)h} - 1 \right) \|v_0\|_W + \left\| \left(e^{-\gamma^-(\cdot)h} - 1 \right) \int_0^t e^{-\gamma^-(\nu)(t-s)} \Lambda^+ v_s ds + \int_t^{t+h} e^{-\gamma^-(\nu)(t+h-s)} \Lambda^+ v_s ds \right\|_W,$$
$$\le \sup_{t\in[0,T]} \left(e^{-\gamma^-(\cdot)h} - 1 \right) \left(\|v_0\|_W + C_W T \sup_{s\in[0,T]} \|v(s,\cdot)\|_W \right) + hC_W \sup_{s\in[t,t+h]} \|v(s,\cdot)\|_W \overset{h\downarrow 0}{\to} 0.$$

Hence, we can conclude $\sup_{t\in[0,T]} \|Tv(t,\cdot)\|_W < \infty$ and $t \mapsto Tv(t,\cdot)$ is continuous. Hence, we can conclude $Tv \in C([0,T];D)$.

Step 5. T is a contraction

To apply Banach Fixed Point Theorem, we require T to be a contraction. We consider the following norm

$$|||w|||_\lambda := \sup_{t\in[0,T]} e^{-\lambda t} \big(\|w(t,\cdot)\|_{L^1} + \|w(t,\cdot)\|_{L^\infty} \big).$$

Let $u_t, v_t \in C([0,T];D)$ with $u_0 = v_0$. For $w_t := u_t - v_t$ it holds that

$$\|Tw(t,\cdot)\|_{L^\infty} \le \operatorname{esssup}_{\nu\in\hat\Gamma_X} \int_0^t \Lambda^+ w_s(\nu)\, ds$$
$$\le C_\infty |||w|||_\lambda \int_0^t e^{\lambda s}\, ds = C_\infty |||w|||_\lambda \frac{1}{\lambda} \big(e^{\lambda t} - 1 \big)$$

Therefore, we have that

$$e^{-\lambda t}\left\|Tw(t,\cdot)\right\|_{L^\infty} \le \frac{C_\infty}{\lambda}\|w\|_\lambda\big(1-e^{-\lambda t}\big).$$

Moreover,

$$\begin{aligned}\left\|Tw(t,\cdot)\right\|_{L^1} &\le \int_{\hat\Gamma_X}\int_0^t \Lambda^+ w_s(\nu)\,ds\,d\hat\Pi^k,\\ &\le C_1\|w\|_\lambda\int_0^t e^{\lambda s}ds = C_1\|w\|_\lambda\frac{1}{\lambda}(e^{\lambda t}-1).\end{aligned}$$

Hence, it holds that

$$e^{-\lambda t}\left\|Tw(t,\cdot)\right\|_{L^1} \le \frac{C_1}{\lambda}\|w\|_\lambda\big(1-e^{-\lambda t}\big).$$

Hence, for $\lambda = C_1 + C_\infty + 1$, the operator T is a contraction with respect to norm $\|\cdot\|_\lambda$. Therefore by Banach Fixed Point Theorem, we can conclude T has a unique fixed point. □

Lemma 4.1.5. If $u \in C([0,T];D)$ is a fixed point of T, then for every $t \in (0,T)$:

$$\left\|\frac{1}{h}\left(u_{t+h}-u_t\right)-\Lambda^+u_t+\gamma^-u_t\right\|_W \to 0. \tag{4.1.20}$$

In particular, u is differentiable at every $t \in (0,T)$ with derivative $u_t' = \Lambda^+u_t - \gamma^-u_t = L_M^* u_t$.

Proof. To show this, we have to show convergence in both the L^1 and the L^∞ norm. We start with the L^1 norm.

We can write $u_{t+h}(\nu) - u_t(\nu)$ as

$$\begin{aligned}&\left(e^{-\gamma^-(\nu)(h)}-1\right)\left(u_0(\nu)-\int_0^t e^{-\gamma^-(\nu)(t-s)}\Lambda^+u_s(\nu)ds\,e^{-\gamma^-(\nu)t}\right)+\int_0^{t+h} e^{-\gamma^-(\nu)(t+h-s)}\Lambda^+u_s(\nu)ds,\\ =&\left(e^{-\gamma^-(\nu)h}-1\right)u_t(\nu)+e^{-\gamma^-(\nu)h}\int_t^{t+h} e^{-\gamma^-(\nu)(t-s)}\Lambda^+u_s(\nu)ds.\end{aligned}$$

Furthermore, we note that

$$\int_{\hat\Gamma_X}\left|\frac{1}{h}\left(e^{-\gamma^-(\nu)h}-1\right)u_t(\nu)-\gamma^-(\nu)u_t(\nu)\right|\hat\Pi^k(d\nu) = \int_{\hat\Gamma_X}\left|\frac{1}{h}\left(e^{-\gamma^-(\nu)h}-1-h\gamma^-(\nu)\right)u_t(\nu)\right|\hat\Pi^k(d\nu).$$

Since $u_t \in L^\infty(\hat\Gamma_X, \hat\Pi^k)$ and $\frac{1}{h}\left(e^{-\gamma^-(\nu)h}-1-h\gamma^-(\nu)\right)$ is also bounded, we can apply Dominated Convergence Theorem to conclude this last expression converges to zero as $h \downarrow 0$.

Moreover, we have that

$$\begin{aligned}&\int_{\hat\Gamma_X}\left|e^{-\gamma^-(\nu)h}\frac{1}{h}\int_t^{t+h} e^{-\gamma^-(\nu)(t-s)}\Lambda^+u_s(\nu)ds-\Lambda^+u_t(\nu)\right|\hat\Pi^k(d\nu)\\ =&\int_{\hat\Gamma_X}\left|\int_0^1 e^{-\gamma^-(\nu)(1-\eta)h}\Lambda^+u_{t+\eta h}(\nu)d\eta-\Lambda^+u_t(\nu)\right|\hat\Pi^k(d\nu),\\ \le&\int_{\hat\Gamma_X}\int_0^1\left|e^{-\gamma^-(\nu)(1-\eta)h}\Lambda^+u_{t+\eta h}(\nu)-\Lambda^+u_t(\nu)\right|d\eta\hat\Pi^k(d\nu).\end{aligned}$$

The second step follows from a change of variables where $s = t + \eta h$.

By applying Fubini's Theorem, we have

$$\begin{aligned}
&\int_{\hat{\Gamma}_X}\int_0^1 \left| e^{-\gamma^-(\nu)(1-\eta)h}\Lambda^+ u_{t+\eta h}(\nu) - \Lambda^+ u_t(\nu)\right| d\eta\, \hat{\Pi}^k(d\nu)\\
&= \int_0^1\int_{\hat{\Gamma}_X} \left| e^{-\gamma^-(\nu)(1-\eta)h}\Lambda^+ u_{t+\eta h}(\nu) - \Lambda^+ u_t(\nu)\right| \hat{\Pi}^k(d\nu)\, d\eta\\
&\leq \int_0^1\int_{\hat{\Gamma}_X} \left(1 - e^{-\gamma^-(\nu)(1-\eta)h}\right)\left|\Lambda^+ u_{t+\eta h}(\nu)\right| \hat{\Pi}^k(d\nu)\, d\eta + \int_0^1 \left\|\Lambda^+ u_{t+\eta h} - \Lambda^+ u_t\right\|_{L^1} d\eta
\end{aligned}$$

The first term converges to zero as $h \downarrow 0$ since $\|\Lambda^+ u_{t+\eta h}\|_{L^\infty} \leq C$ uniformly in h, and it holds that

$$1 - e^{-\gamma^-(\nu)(1-\eta)h} \overset{h\downarrow 0}{\to} 0 \quad \text{for } \hat{\Pi}^k\text{-almost every } \nu.$$

Moreover, Λ^+ is linear and bounded. Hence, there exists some C_Λ such that

$$\left\|\Lambda^+ u_{t+\eta h} - \Lambda^+ u_t\right\|_{L^1} \leq C_\Lambda \left\|u_{t+\eta h} - u_t\right\|_{L^1}.$$

This last expression converges to zero, because u_t is continuous in L^1. Applying the dominated convergence, we then deduce that the earlier expression converges to zero. Hence, we conclude that

$$\left\|\frac{1}{h}\left(u_{t+h} - u_t\right) - \Lambda^+ u_t + \gamma^- u_t\right\|_{L^1} \to 0.$$

In similar fashion we obtain the convergence in the L^∞-norm.

Altogether, we find that indeed

$$\left\|\frac{1}{h}\left(u_{t+h} - u_t\right) - \Lambda^+ u_t + \gamma^- u_t\right\|_W \to 0. \tag{4.1.21}$$

□

Due to our reformulation into a fixed point problem we know that any solution of (4.1.1) is a fixed point of operator T as defined in (4.1.19). So far we proved existence and uniqueness of a fixed point of T. Moreover, we proved that a fixed point of T satisfies (4.1.20). To establish existence and uniqueness of a solution of system (4.1.1), we still have to show that a fixed point of T is indeed a mild solution of (4.1.1). To prove this, we use that a fixed point of T must satisfy (4.1.20). This result is stated in the following lemma.

Lemma 4.1.6. Let $u \in C([0,T];D)$ be a fixed point of T given by (4.1.19). Then u_t is a mild solution of system (4.1.1).

Proof. This proof consists of two steps. First, we show u_t is absolutely continuous in L^p spaces with $p \in (1,\infty)$. From this we conclude there exists a function $g(s)$ such that $u_t = u_0 + \int_0^t g(s)ds$ in L^p by application of Lemma 4.1.2. In the second step, we show $g(s) = L_M^* u_s$ almost everywhere.

Step 1. Absolute continuity

Let $p \in (1,\infty)$. Let $0 \leq t < t+h \leq T$. It holds that

$$\begin{aligned}
\|u_{t+h} - u_t\|_{L^p} &= \left\|\left(e^{-\gamma^-(\cdot)h} - 1\right)u_t + e^{-\gamma^-(\cdot)h}\int_t^{t+h} e^{-\gamma^-(\cdot)(t-r)}\Lambda^+ u_r dr\right\|_{L^p}\\
&= \left\|\int_t^{t+h} \frac{1}{h}\left(e^{-\gamma^-(\cdot)h} - 1\right)u_t + e^{-\gamma^-(\cdot)(t+h-r)}\Lambda^+ u_r dr\right\|_{L^p}\\
&\leq \int_t^{t+h} \left\|\frac{1}{h}\left(e^{-\gamma^-(\cdot)h} - 1\right)u_t + e^{-\gamma^-(\cdot)(t+h-r)}\Lambda^+ u_r\right\|_{L^p} dr.
\end{aligned}$$

We note that $\|u_t\|_{L^p} \leq \|u_t\|_{L^\infty}^{p-1} \|u_t\|_{L^1} < \infty$. Similarly, since Λ^+ is bounded in W, it holds that $\|\Lambda^+ u_s\|_{L^p} < \infty$. Moreover, for $h > 0$, it holds that $\left\| \frac{1}{h} \left(e^{-\gamma^-(\cdot)h} - 1 \right) \right\|_{L^p} < \infty$. This means we can conclude that u is absolutely continuous. Since the space L^p is reflexive for $p \in (1, \infty)$, we conclude by Lemma 4.1.2 that $u : [0,T] \to L^p(\hat{\Gamma}_X, \hat{\Pi}^k)$ is differentiable almost everywhere and there exists a function $g(s)$ such that the following equality holds in L^p

$$u_t = u_0 + \int_0^t g(s)ds \qquad \forall t \in [0,T]. \tag{4.1.22}$$

Step 2. Equality almost everywhere
From equality (4.1.22), we derive that

$$\frac{u_{t+h}(\nu) - u_t(\nu)}{h} = \frac{1}{h} \int_t^{t+h} g(s)ds.$$

Since $L_M^* u_t \in W$, we again conclude $L_M^* u_t \in L^p$. Moreover, $g \in L^p$. Therefore, due to finiteness of measure $\hat{\Pi}^k$, we find by applying the Dominated Convergence Theorem that

$$\left\| \frac{u_{t+h} - u_t}{h} - L_M^* u_t \right\|_{L^p} \overset{h \downarrow 0}{\to} \|g(t) - L_M^* u_t\|_{L^p}.$$

Moreover,

$$\left\| \frac{u_{t+h} - u_t}{h} - L_M^* u_t \right\|_{L^p} \leq \left\| \frac{u_{t+h} - u_t}{h} - L_M^* u_t \right\|_W \to 0.$$

Hence, for all $p \in (1, \infty)$, we have

$$\|g(t) - L_M^* u_t\|_{L^p} = 0.$$

Therefore, we conclude $g(t) = L_M^* u_t$ almost everywhere. □

We found a solution u_t^M to system (4.1.1). However, we started with a formulation of the forward Kolmogorov equation in terms of a probability measure ρ_t^M. We made the assumption that u_t^M is the Radon-Nikodym derivative of this probability measure ρ_t^M. We can define $\rho_t^M(d\nu) := u_t^M(\nu) d\hat{\Pi}^k(d\nu)$, but we still want to check that this is indeed a probability measure. This happens in the next lemma.

Lemma 4.1.7. Let u_t^M be a solution of system (4.1.1) with $\int_{\hat{\Gamma}_X} u_0^M d\hat{\Pi}^k(\nu) = 1$. Then $\int_{\hat{\Gamma}_X} u_t^M d\hat{\Pi}^k(\nu) = 1$ for all $t \geq 0$.

Proof. Since u_t^M is a solution of (4.1.1), we know

$$u_t^M = u_0^M + \int_0^t L_M^* u_s^M ds.$$

Hence,

$$\begin{aligned} \int_{\hat{\Gamma}_X} u_t^M(\nu) d\hat{\Pi}^k &= \int_{\hat{\Gamma}_X} u_0^M(\nu) d\hat{\Pi}^k + \int_{\hat{\Gamma}_X} \int_0^t L_M^* u_s^M(\nu) ds d\hat{\Pi}^k, \\ &= 1 + \int_{\hat{\Gamma}_X} \int_0^t L_M^* u_s^M(\nu) ds d\hat{\Pi}^k \end{aligned}$$

We want to prove that $\int_{\hat{\Gamma}_X} \int_0^t L_M^* u_s^M(\nu) d\hat{\Pi}^k = 0$.

By Fubini's Theorem we have

$$\int_{\hat{\Gamma}_X} \int_0^t L_M^* u_s^M(\nu) ds d\hat{\Pi}^k = \int_0^t \int_{\hat{\Gamma}_X} L_M^* u_s^M(\nu) d\hat{\Pi}^k ds.$$

When we consider the inner integral for the birth part, we find

$$\begin{aligned}\int_{\hat{\Gamma}_X} L_{M,\beta}^* u_s^M(\nu) d\hat{\Pi}^k &= \int_{\hat{\Gamma}_X} \sum_{m=1}^{k} \left(\sum_{x \in \nu_m} \kappa_{0m}^M(x, \nu - \delta_x e_m) u_s^M(\nu - \delta_x e_m) - \kappa_{0m}^M(X, \nu) u_s^M(\nu) \right) d\hat{\Pi}^k, \\ &= \int_{\hat{\Gamma}_X} \sum_{m=1}^{k} \left(\kappa_{0m}^M(X, \nu) u_s^M(\nu) - \kappa_{0m}^M(X, \nu) u_s^M(\nu) \right) d\hat{\Pi}^k = 0.\end{aligned}$$

This follows from application of Lemma 3.1.1, where $F(\nu) = 1$ for all $\nu \in \hat{\Gamma}_X$. The computations for the transition and the death part work analogously. □

Chapter 5

Weak solution to the forward Kolmogorov equation

5.1 Moment bounds

In Theorem 4.1.4, we proved that the truncated system (4.1.1) is well-posed. Since the evolution operator in this system depends on M, we want to extend this result to establish existence of a solution to the original forward Kolmogorov equation. In Sections 5.1 and 5.2, we prove a priori estimates that are essential for the proof of existence. For the moment bounds, we look at state space Γ_X, which is defined as follows

$$\Gamma_X := \left[\mathcal{M}^+(X)\right]^k. \tag{5.1.1}$$

We consider the measure Π^k on this set Γ_X as introduced in Chapter 2.

Lemma 5.1.1. Let $T > 0$ and let ρ_t^M be a solution to (4.1.1) for every $M \in \mathbb{N}$. Then there exists a constant $B_1 > 0$ such that for all $t \in [0, T]$

$$\int_{\Gamma_X} \|\nu\|_{TV}\, \rho_t^M(d\nu) \leq \left(\int_{\Gamma_X} \|\nu\|_{TV}\, \rho_0^M(d\nu) \right) e^{B_1 T}$$

This implies that there exists a constant $c_1 > 0$ independent of M, such that

$$c_1 := \sup_{t\in[0,T], M\in\mathbb{N}} \int_{\Gamma_X} \|\nu\|_{TV}\, \rho_t^M(d\nu) < \infty. \tag{5.1.2}$$

Furthermore, there exists a constant C_L:

$$C_L := 2\overline{\kappa}\left(C_\beta k + \binom{k}{2} + k \right). \tag{5.1.3}$$

such that for all $t, s \in [0, T]$, we have

$$|\langle F, \rho_t^M \rangle - \langle F, \rho_s^M \rangle| \leq c_1 C_L \|F\|_{\sup} |t - s|. \tag{5.1.4}$$

Proof. First, we consider functions $F_p(\nu), p \in \mathbb{N}$ of the form $F_p(\nu) = \min\{p, \|\nu\|_{TV}\}$. The functions $F_p(\nu)$ are continuous and bounded for all $p \in \mathbb{N}$. Furthermore, for these type of functions, we know for all $i, j \in \{1, \ldots, k\}, i \neq j$, that

$$|F_p(\nu - \delta_x e_i + \delta_x e_j) - F_p(\nu)| = 0.$$

Moreover, for all $m \in \{1, \dots, k\}$, we have

$$|F_p(\nu + \delta_y e_m) - F_p(\nu)| \le \mathbb{1}_{\|\nu\|_{TV} \le p},$$

and for all $l \in \{1, \dots, k\}$, it holds that

$$|F_p(\nu - \delta_y e_l) - F_p(\nu)| \le \mathbb{1}_{\|\nu\|_{TV} \le p}.$$

Hence, for the birth part, we have

$$\begin{aligned}
\left|\langle L_\beta^M F_p, \rho_r^M(d\nu)\rangle\right| &= \left| \int_{\Gamma_X} \sum_{m=1}^k \int_X \left[F_p(\nu + \delta_y e_m) - F_p(\nu)\right] \kappa_{0m}^M(y, \nu)\lambda(dy)\rho_r^M(d\nu) \right|, \\
&\le \int_{\Gamma_X} \sum_{m=1}^k \mathbb{1}_{\|\nu\|_{TV} \le p} \left|\kappa_{0m}^M(X, \nu)\right| \rho_r^M(d\nu), \\
&\le C_\beta \overline{\kappa} \int_{\Gamma_X} \sum_{m=1}^k \mathbb{1}_{\|\nu\|_{TV} \le p} \|\nu_m\|_{TV} \, \rho_r^M(d\nu), \\
&\le k\overline{\kappa} C_\beta \int_{\Gamma_X} F_p(\nu)\rho_r^M(d\nu).
\end{aligned}$$

Furthermore, for the death part, we have

$$\begin{aligned}
\left|\langle L_\delta^M F_p, \rho_r^M(d\nu)\right| &= \left| \int_{\Gamma_X} \sum_{l=1}^k \sum_{x \in \nu_l} \left[F(\nu - \delta_x e_l) - F(\nu)\right] \kappa_{l0}^M(x, \nu)\rho_r^M(d\nu) \right|, \\
&\le \int_{\Gamma_X} \sum_{l=1}^k \mathbb{1}_{\|\nu\|_{TV} \le p} \sum_{x \in \nu_l} |\kappa_{l0}^M(x, \nu)| \rho_r^M(d\nu), \\
&\le \sum_{l=1}^k \overline{\kappa} \int_{\Gamma_X} \mathbb{1}_{\|\nu\|_{TV} \le p} \|\nu_l\|_{TV} \, \rho_r^M(d\nu), \\
&\le k\overline{\kappa} \int_{\Gamma_X} F_p(\nu)\rho_r^M(d\nu).
\end{aligned}$$

We define $B_1 := k\overline{\kappa}C_\beta + k\overline{\kappa}$, then we know

$$\begin{aligned}
\langle F_p, \rho_t^M\rangle &= \langle F_p, \rho_0^M\rangle + \int_0^t \langle L^M F_p, \rho_r^M\rangle dr, \\
&\le \langle F_p, \rho_0^M\rangle + B_1 \int_0^t \int_{\Gamma_X} F_p(\nu)\rho_r^M(d\nu)dr.
\end{aligned}$$

Therefore, by Gronwall's inequality, we can conclude

$$\int_{\Gamma_X} F_p(\nu)\rho_t^M(d\nu) \le \left(\int_{\Gamma_X} F_p(\nu)\rho_0^M(d\nu) \right) e^{B_1 T} \qquad \text{for all } t \in [0, T].$$

Therefore, by the Monotone Convergence Theorem, we have

$$\int_{\Gamma_X} \|\nu\|_{TV} \, \rho_t^M(d\nu) \le \left(\int_{\Gamma_X} \|\nu\|_{TV} \, \rho_0^M(d\nu) \right) e^{B_1 T} \qquad \text{for all } t \in [0, T].$$

Hence, we can conclude

$$c_1 := \sup_{t \in [0,T], M \in \mathbb{N}} \int_{\Gamma_X} \|\nu\|_{TV} \, \rho_t^M(d\nu) < \infty.$$

Let $s, t \in [0,T]$. Then

$$|\langle F, \rho_t^M\rangle - \langle F, \rho_s^M\rangle| \leq \int_s^t |\langle L^M F, \rho_r^M\rangle| dr \leq \int_s^t |\langle L_\beta^M F, \rho_r^M\rangle| + |\langle L_\tau^M F, \rho_r^M\rangle| + |\langle L_\delta^M F, \rho_r^M\rangle| dr.$$

We have

$$\begin{aligned}|\langle L_\beta^M F, \rho_r^M\rangle| &\leq \int_{\Gamma_X} \left| \sum_{m=1}^k \int_X [F(\nu + \delta_y e_m) - F(\nu)] \kappa_{0m}^M(y,\nu)\lambda(dy) \right| \rho_r^M(d\nu), \\ &\leq 2k\overline{\kappa} C_\beta \|F\|_{\sup} \int_{\Gamma_X} \|\nu\|_{TV}\, \rho_r^M(d\nu).\end{aligned}$$

Moreover,

$$\begin{aligned}|\langle L_\tau^M F, \rho_r^M\rangle| &\leq \int_{\Gamma_X} \left| \sum_{i,j\neq i} \sum_{x\in\nu_i} [F(\nu - \delta_x e_i + \delta_x e_j) - F(\nu)] \kappa_{ij}^M(x,\nu) \right| \rho_r^M(d\nu), \\ &\leq 2\binom{k}{2} \overline{\kappa} \|F\|_{\sup} \int_{\Gamma_X} \|\nu\|_{TV}\, \rho_r^M(d\nu).\end{aligned}$$

Lastly,

$$\begin{aligned}|\langle L_\delta^M F, \rho_r^M\rangle| &\leq \int_{\Gamma_X} \left| \sum_{l=1}^k \sum_{x\in\nu_l} [F(\nu - \delta_y e_l) - F(\nu)] \kappa_{l0}^M(x,\nu) \right| \rho_r^M(d\nu), \\ &\leq 2k\overline{\kappa} \|F\|_{\sup} \int_{\Gamma_X} \|\nu\|_{TV}\, \rho_r^M(d\nu).\end{aligned}$$

Hence, it holds that

$$|\langle F, \rho_t^M\rangle - \langle F, \rho_s^M\rangle| \leq \int_s^t C_L\, \|F\|_{\sup} \int_{\Gamma_X} \|\nu\|_{TV}\, \rho_r^M(d\nu) dr \leq c_1 C_L \|F\|_{\sup} |t-s|.$$

□

The calculations made in Lemma 5.1.1 also work for higher order moments. We explicitly show this for the second moment.

Lemma 5.1.2. Let $T > 0$ and let, for every $M \in \mathbb{N}$, ρ_t^M be a solution to (4.1.1). Then there exists a constant B_2 such that

$$\int_{\Gamma_X} \|\nu\|_{TV}^2\, \rho_t^M(d\nu) \leq \int_{\Gamma_X} \|\nu\|_{TV}^2\, \rho_0^M(d\nu) e^{B_2 t} \qquad \text{for all } t \in [0,T]$$

This implies that

$$c_2 := \sup_{t\in[0,T], M\in\mathbb{N}} \int_{\Gamma_X} \|\nu\|_{TV}^2\, \rho_t^M(d\nu) < \infty. \tag{5.1.5}$$

Proof. First, we consider functions $F_p(\nu), p \in \mathbb{N}$ of the form $F_p(v) = \min\{p, \|\nu\|_{TV}^2\}$. The functions $F_p(\nu)$ are continuous and bounded for all $p \in \mathbb{N}$. Furthermore, for these type of functions, we know for all $i, j \in \{1, \dots, k\}, i \neq j$, that

$$|F_p(\nu - \delta_x e_i + \delta_x e_j) - F_p(\nu)| = 0.$$

Moreover, for all $m \in \{1, \ldots, k\}$, we have

$$|F_p(\nu + \delta_y e_m) - F_p(\nu)| \leq (2\|\nu\|_{TV} + 1)\mathbb{1}_{\|\nu\|^2_{TV} \leq p},$$

and for all $l \in \{1, \ldots, k\}$, it holds that

$$|F_p(\nu - \delta_y e_l) - F_p(\nu)| \leq (2\|\nu\|_{TV} + 1)\mathbb{1}_{\|\nu\|^2_{TV} \leq p}.$$

Hence, for the birth part it holds that

$$\begin{aligned}
\left|\langle L^M_\beta F_p, \rho^M_r\rangle\right| &= \left|\int_{\Gamma_X} \sum_{m=1}^{k} \int_X \left[F_p(\nu + \delta_y e_m) - F_p(\nu)\right] \kappa^M_{0m}(\nu, y)]\lambda(dy)\rho^M_r(d\nu)\right|, \\
&\leq \int_{\Gamma_X} \sum_{m=1}^{k} (2\|\nu\|_{TV} + 1)\mathbb{1}_{\|\nu\|^2_{TV} \leq p}\left|\kappa^M_{0m}(\nu, X)\right|\rho^M_r(d\nu), \\
&\leq C_\beta \overline{\kappa} \int_{\Gamma_X} \sum_{m=1}^{k} (2\|\nu\|_{TV} + 1)\mathbb{1}_{\|\nu\|^2_{TV} \leq p} \|\nu_m\|_{TV} \rho^M_r(d\nu), \\
&\leq 3k\overline{\kappa}C_\beta \int_{\Gamma_X} \|\nu\|^2_{TV} \rho^M_r(d\nu), \\
&\leq 3k\overline{\kappa}C_\beta \int_{\Gamma_X} F_p(\nu)\rho^M_r(d\nu).
\end{aligned}$$

For the death part, it holds that

$$\begin{aligned}
\left|\langle L^M_\delta F_p, \rho^M_r\rangle\right| &= \left|\sum_{l=1}^{k} \sum_{x \in \nu_l} \left[F(\nu - \delta_x e_l) - F(\nu)\right] \kappa^M_{l0}(x, \nu)\rho^M_r(d\nu)\right|, \\
&\leq \sum_{l=1}^{k} (2\|\nu\|_{TV} + 1)\mathbb{1}_{\|\nu\|^2_{TV} \leq p} \sum_{x \in \nu_l} |\kappa^M_{l0}(x, \nu)|\rho^M_r(d\nu), \\
&\leq \sum_{l=1}^{k} \overline{\kappa}(2\|\nu\|_{TV} + 1)\mathbb{1}_{\|\nu\|^2_{TV} \leq p} \|\nu_l\|_{TV} \rho^M_r(d\nu), \\
&\leq 3k\overline{\kappa} \int_{\Gamma_X} \|\nu\|^2_{TV} \rho^M_r(d\nu), \\
&\leq 3k\overline{\kappa} \int_{\Gamma_X} F_p(\nu)\rho^M_r(d\nu).
\end{aligned}$$

We define $B_2 := 3k\overline{\kappa}(C_\beta + 1)$, then we know

$$\begin{aligned}
\langle F_p, \rho^M_t\rangle &= \langle F_p, \rho^M_0\rangle + \int_0^t \langle L^M F_p, \rho^M_r\rangle dr, \\
&\leq \langle F_p, \rho^M_0\rangle + B_2 \int_0^t \int_{\Gamma_X} F_p(\nu)\rho^M_r(d\nu)dr.
\end{aligned}$$

Therefore, by Gronwall's inequality, we can conclude

$$\int_{\Gamma_X} F_p(\nu)\rho^M_t(d\nu) \leq \left(\int_{\Gamma_X} F_p(\nu)\rho^M_0(d\nu)\right) e^{B_2 T} \qquad \text{for all } t \in [0, T].$$

Therefore, by the Monotone Convergence Theorem, we have

$$\int_{\Gamma_X} \|\nu\|^2_{TV} \rho^M_t(d\nu) \leq \left(\int_{\Gamma_X} \|\nu\|^2_{TV} \rho^M_0(d\nu)\right) e^{B_2 T} \qquad \text{for all } t \in [0, T].$$

Hence,

$$c_2 := \sup_{t\in[0,T], M\in\mathbb{N}} \int_{\Gamma_X} \|\nu\|_{TV}^2 \, \rho_t^M(d\nu) < \infty.$$

□

5.2 Entropy inequality

Next, we want to find a bound of the Boltzmann entropy functional. Based on [13], we define this entropy functional as follows.

Definition 5.2.1. The entropy functional is given by

$$\mathsf{Ent}(\rho|\hat{\Pi}^k) := \begin{cases} \int_{\Gamma_X} \phi(u(\nu)) d\hat{\Pi}^k(\nu) & \text{if } \rho \ll \hat{\Pi}^k \text{ with } u = \frac{d\rho}{d\hat{\Pi}^k}, \\ +\infty & \text{otherwise,} \end{cases}$$

where $\phi(s) := s\log(s) - s + 1$ is called the Boltzmann entropy function.

Note that a finite bound on this entropy functional implies that ρ is absolutely continuous with respect to $\hat{\Pi}^k$. In Theorem 5.4.2, this implication is used in the proof. First, however, we want to prove the entropy functional is differentiable and determine a bound of the entropy functional.

Lemma 5.2.2. Let for each $M \in \mathbb{N}$, u_t^M be a solution to truncated forward Kolmogorov equation (4.1.1), with $\int_{\hat{\Gamma}_X} u_0^M d\hat{\Pi}^k = 1$. Define $\rho_t^M = u_t^M d\hat{\Pi}^k$ and assume that $\mathsf{Ent}(\rho_0^M|\hat{\Pi}^k) < \infty$. Then $\mathsf{Ent}(\rho_t^M|\hat{\Pi}^k)$ is differentiable. Moreover,

$$\mathsf{Ent}(\rho_t^M|\hat{\Pi}^k) \le \mathsf{Ent}(\rho_0^M|\hat{\Pi}^k) + c_{\mathsf{Ent}} t, \tag{5.2.1}$$

where $c_{\mathsf{Ent}} := c_1\overline{\kappa}\left(k + \binom{k}{2} + kC_\delta\right)$.

Proof. The proof of differentiability is based on the proof of Theorem 4.16 from [13].
Let $\ell \in \mathbb{N}$ and let $\phi_\ell'(\sigma) := \min\{\log(\sigma + \ell^{-1}), \ell\}$. Then we define $\phi_\ell(s) = \int_0^s \phi_\ell'(\sigma)d\sigma$. We note that this $\phi_\ell'(\sigma)$ is concave and monotonically increasing. This latter property implies $\phi_\ell(s)$ is convex. Furthermore, we define

$$S_\ell(t) := \int_{\hat{\Gamma}_X} \phi_\ell(u_t^M) d\hat{\Pi}^k,$$
$$S(t) := \int_{\hat{\Gamma}_X} \phi(u_t^M) d\hat{\Pi}^k.$$

Furthermore, we have

$$\begin{aligned} S_\ell(t) - S_\ell(s) &= \int_{\hat{\Gamma}_X} \left[\phi_\ell(u_t^M) - \phi_\ell(u_s^M)\right] d\hat{\Pi}^k, \\ &= \int_{\hat{\Gamma}_X} \left(\int_0^1 \phi_\ell'((1-\lambda)u_s^M + \lambda u_t^M)\, d\lambda\right) \left[u_t^M - u_s^M\right] d\hat{\Pi}^k \\ &\le \ell \int_{\hat{\Gamma}_X} \left|u_t^M(\nu) - u_s^M(\nu)\right| d\hat{\Pi}^k \\ &= \ell \int_{\hat{\Gamma}_X} \left|\int_s^t \partial_r u_r^M dr\right| d\hat{\Pi}^k, \\ &\le \ell \int_{\hat{\Gamma}_X} \int_s^t \left|\partial_r u_r^M\right| dr d\hat{\Pi}^k, \\ &= \ell \int_s^t \int_{\hat{\Gamma}_X} \left|\partial_r u_r^M\right| d\hat{\Pi}^k dr. \end{aligned}$$

We note that $\int_{\hat{\Gamma}_X} |\partial_r u_r^M| d\hat{\Pi}^k < \infty$, since $\partial_r u_r^M = L^{M*} u_r^M$ and we know this is an L^1-function. Therefore, the mapping $t \mapsto S_\ell(t)$ is absolutely continuous and this implies differentiability almost everywhere

Next, we want to investigate this limit. Let $t \in (0,T)$. We know u_t^M is continuous in L^1 with respect to t. Therefore, we know there exists a subsequence $(h_n)_{n\in\mathbb{N}}$ such that $u_{t+h_n}^M$ is pointwise continuous almost everywhere.

It holds that

$$\begin{aligned}\frac{S_\ell(t+h_n) - S_\ell(t)}{h_n} &= \int_{\hat{\Gamma}_X} \left(\int_0^1 \phi_\ell'((1-\lambda)u_t^M(\nu) + \lambda u_{t+h_n}^M(\nu))\, d\lambda \right) \frac{u_{t+h_n}^M(\nu) - u_t^M(\nu)}{h_n}\, d\hat{\Pi}^k, \\ &= \frac{1}{h_n} \int_{\hat{\Gamma}_X} \left(\int_0^1 \phi_\ell'((1-\lambda)u_t^M(\nu) + \lambda u_{t+h_n}^M(\nu))\, d\lambda \right) \int_t^{t+h_n} L_M^* u_r^M(\nu)\, dr\, d\hat{\Pi}^k.\end{aligned}$$

Here, the first step is an application of the definition and the fundamental theorem of calculus. The second step is an application of the definition of L_M^*. Applying Fubini's Theorem, we get

$$\begin{aligned}\frac{S_\ell(t+h^n) - S_\ell(t)}{h^n} &= \frac{1}{h^n} \int_t^{t+h^n} \int_{\hat{\Gamma}_X} \left(\int_0^1 \phi_\ell'((1-\lambda)u_t^M(\nu) + \lambda u_{t+h^n}^M(\nu))\, d\lambda \right) L_M^* u_r^M(\nu)\, d\hat{\Pi}^k\, dr, \\ &= \int_0^1 \int_{\hat{\Gamma}_X} \left(\int_0^1 \phi_\ell'((1-\lambda)u_t^M(\nu) + \lambda u_{t+h^n}^M(\nu))\, d\lambda \right) L_M^* u_{t+\eta h^n}^M(\nu)\, d\hat{\Pi}^k\, d\eta,\end{aligned}$$

In the previous step, we applied a change of variables on r. Moreover, due to the boundedness of ϕ_ℓ', we know the integral $\left(\int_0^1 \phi_\ell'((1-\lambda)u_t^M(\nu) + \lambda u_{t+h_n}^M(\nu))\, d\lambda \right)$ is bounded. We also know that $u_t^M(\nu)$ is in L^∞ for all t. Hence,

$$|L_M^* u_{t+\eta h^n}^M(\nu)| \le 2M\overline{\kappa} \left(C_\beta k + \binom{k}{2} + C_\delta k \right) \sup_{s\in[t,t+h]} \left\| u^M(s,\cdot) \right\|_{L^\infty} < \infty.$$

Hence, due to L_∞ bound and the finiteness of measure $\hat{\Pi}^k$ there exists a dominating function and we can use the Dominated Convergence Theorem, to conclude

$$\frac{S_\ell(t+h_n) - S_\ell(t)}{h_n} \overset{h_n\downarrow 0}{\to} \int_{\hat{\Gamma}_X} \phi_\ell'(u_t^M(\nu)) L_M^* u_t^M(\nu)\, d\hat{\Pi}^k.$$

Hence, we have that

$$\begin{aligned}\frac{d}{dt} S_\ell(t) &= \int_{\hat{\Gamma}_X} \phi_\ell'(u_t^M) L_M^* u_t^M d\hat{\Pi}^k, \\ &= \int_{\hat{\Gamma}_X} L^M(\phi_\ell'(u_r^M)) u_r^M d\hat{\Pi}^k dr, \\ &= \int_{\hat{\Gamma}_X} \left(\left(L^M(\phi_\ell'(u_r^M)\right)_+ u_r^M - \left(L^M(\phi_\ell'(u_r^M)\right)_- u_r^M \right) d\hat{\Pi}^k, \\ &\le \int_{\hat{\Gamma}_X} \left(L^M(\phi_\ell'(u_r^M)\right)_+ u_r^M\, d\hat{\Pi}^k.\end{aligned}$$

We want to find a uniform estimate for $\int_s^t \int_{\hat{\Gamma}_X} \left(L^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k$.

$$\int_{\hat{\Gamma}_X} \left(L^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k \le \int_{\hat{\Gamma}_X} \left(\left(L_\beta^M(\phi_\ell'(u_r^M)\right)_+ + \left(L_\tau^M(\phi_\ell'(u_r^M)\right)_+ + \left(L_\delta^M(\phi_\ell'(u_r^M)\right)_+ \right) u_r^M d\hat{\Pi}^k.$$

We have that

$$\int_{\hat{\Gamma}_X} \left(L_\beta^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k \leq \int_{\hat{\Gamma}_X} \sum_{m=1}^k \int_X \left(\phi_\ell'(u_t^M(\nu+\delta_y e_m)) - \phi_\ell'(u_t^M(\nu))\right)_+ \kappa_{0m}^M(y,\nu)\lambda(dy).$$

Since the function ϕ_ℓ' is concave, we know that

$$\begin{aligned}\left(\phi_\ell'(u_t^M(\nu+\delta_y e_m)) - \phi_\ell'(u_t^M(\nu))\right)_+ &\leq \phi_\ell''(u_t^M(\nu))\left(u_t^M(\nu+\delta_y e_m) - u_t^M(\nu)\right)_+, \\ &= \frac{1}{u_t^M(\nu)+\ell^{-1}}\left(u_t^M(\nu+\delta_y e_m) - u_t^M(\nu)\right)_+ \mathbb{1}_{\phi_\ell'(u_t^M(\nu))\leq \ell}.\end{aligned}$$

Since the rate functions and $u_t^M(\nu)$ are nonnegative, we can conclude

$$\begin{aligned}\int_{\hat{\Gamma}_X} \left(L_\beta^M(\phi_\ell'(u_t^M)\right)_+ u_t^M d\hat{\Pi}^k &\leq \int_{\hat{\Gamma}_X} \sum_{m=1}^k \frac{u_t^M(\nu)}{u_t^M(\nu)+\ell^{-1}} \int_X \left(u_t^M(\nu+\delta_y e_m) - u_t^M(\nu)\right)_+ \kappa_{0m}^M(y,\nu)\lambda(dy)d\hat{\Pi}^k, \\ &\leq \int_{\hat{\Gamma}_X} \sum_{m=1}^k \int_X u_t^M(\nu+\delta_y e_m)\kappa_{0m}^M(y,\nu)\lambda(dy)d\hat{\Pi}^k.\end{aligned}$$

By application of Lemma 3.1.1, we find

$$\int_{\hat{\Gamma}_X} \left(L_\beta^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k \leq \int_{\hat{\Gamma}_X} u_r^M(\nu) \sum_{m=1}^k \sum_{x\in\nu_m} \kappa_{0m}^M(x,\nu-\delta_x e_m)d\hat{\Pi}^k \leq k\overline{\kappa}\int_{\hat{\Gamma}_X} \|\nu\|_{TV}\,\rho_r^M(d\nu).$$

Similarly, for the transition part of the operator L^M, it holds that

$$\left(L_\tau^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k(\nu) \leq \sum_{i,j\neq i}\sum_{x\in\nu_i} \left(\phi_\ell'(u_t^M(\nu-\delta_x e_i+\delta_x e_j)) - \phi_\ell'(u_t^M(\nu))\right)_+ \kappa_{ij}^M(x,\nu)u_r^M d\hat{\Pi}^k.$$

Due to concaveness, we find

$$\begin{aligned}\left(\phi_\ell'(u_t^M(\nu-\delta_x e_i+\delta_x e_j)) - \phi_\ell'(u_t^M(\nu))\right)_+ &\leq \phi_\ell''(u_t^M(\nu))\left(u_t^M(\nu-\delta_x e_i+\delta_x e_j) - u_t^M(\nu)\right)_+, \\ &= \frac{1}{u_t^M(\nu)+\ell^{-1}}\left(u_t^M(\nu-\delta_x e_i+\delta_x e_j) - u_t^M(\nu)\right)_+ \mathbb{1}_{\phi_\ell'\leq \ell}.\end{aligned}$$

Hence, we can conclude

$$\begin{aligned}\left(L_\tau^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k(\nu) &\leq \int_{\hat{\Gamma}_X} \sum_{i,j\neq i} \frac{u_r^M(\nu)}{u_r^M(\nu)+\ell^{-1}} \sum_{x\in\nu_i} \kappa_{ij}^M(x,\nu)\left(u_r^M(\nu-\delta_x e_i+\delta_x e_j) - u_r^M(\nu)\right)_+ d\hat{\Pi}^k, \\ &\leq \int_{\hat{\Gamma}_X} \sum_{i,j\neq i}\sum_{x\in\nu_i} u_r^M(\nu-\delta_x e_i+\delta_x e_j)\kappa_{ij}^M(x,\nu)d\hat{\Pi}^k.\end{aligned}$$

Again, by application of Lemma 3.1.1, we find

$$\left(L_\tau^M(\phi_\ell'(u_r^M)\right)_+ u_r^M(\nu) d\hat{\Pi}^k \leq \int_{\hat{\Gamma}_X} \sum_{i,j\neq i}\sum_{x\in\nu_j} \kappa_{ij}^M(x,\nu+\delta_x e_i-\delta_x e_j)u_r^M(\nu)\hat{\Pi}^k \leq \binom{k}{2}\overline{\kappa}\int_{\hat{\Gamma}_X} \|\nu\|_{TV}\,\rho_r^M(d\nu).$$

Lastly, for the death part of the operator, we get

$$\int_{\hat{\Gamma}_X} \left(L_\delta^M(\phi_\ell'(u_r^M)\right)_+ u_r^M d\hat{\Pi}^k \leq \int_{\hat{\Gamma}_X} \sum_{l=1}^k \sum_{x\in\nu_l} \left(\phi_\ell'(u_t^M(\nu-\delta_x e_l) - \phi_\ell'(u_t^M(\nu))\right)_+ \kappa_{l0}^M(x,\nu)u_r^M(\nu)d\hat{\Pi}^k(\nu).$$

Moreover,

$$\begin{aligned}\left(\phi_\ell'(u_t^M(\nu-\delta_x e_l))-\phi_\ell'(u_t^M(\nu))\right)_+ &\le \phi_\ell''(u_t^M(\nu))\left(u_t^M(\nu-\delta_x e_l)-u_t^M(\nu)\right)_+,\\ &= \frac{1}{u_t^M(\nu)+\ell^{-1}}\left(u_t^M(\nu-\delta_x e_l)-u_t^M(\nu)\right)_+ \mathbb{1}_{\phi_\ell'\le\ell}.\end{aligned}$$

Hence, we can conclude

$$\begin{aligned}\int_{\hat\Gamma_X}\left(L_\delta^M(\phi_\ell'(u_r^M))\right)_+ u_r^M d\hat\Pi^k(\nu) &\le \int_{\hat\Gamma_X}\sum_{l=1}^k \frac{u_r^M(\nu)}{u_r^M(\nu)+\ell^{-1}}\sum_{x\in\nu_l}\left(u_r^M(\nu-\delta_x e_l)-u_r^M(\nu)\right)_+\kappa_{l0}^M(x,\nu)d\hat\Pi^k(\nu),\\ &\le \int_{\hat\Gamma_X}\sum_{l=1}^k\sum_{x\in\nu_l}u_r^M(\nu-\delta_x e_l)\kappa_{l0}^M(x,\nu)d\hat\Pi^k(\nu),\end{aligned}$$

By application of Lemma 3.1.1, we find

$$\left(L_\delta^M(\phi_\ell'(u_r^M))\right)_+ u_r^M d\hat\Pi^k(\nu)\le \int_{\hat\Gamma_X}\sum_{l=1}^k\int_X \kappa_{l0}(y,\nu+\delta_y e_l)\lambda(dy)u_r^M(\nu)d\hat\Pi^k \le k\overline{\kappa}C_\delta\int_{\hat\Gamma_X}\|\nu\|_{TV}\,\rho_r^M(d\nu).$$

Combining these bounds, we find

$$\int_{\hat\Gamma_X}\left(L^M(\phi_\ell'(u_r^M))\right)_+ u_r^M d\hat\Pi^k \le \overline{\kappa}\left(k+\binom{k}{2}+kC_\delta\right)\int_{\hat\Gamma_X}\|\nu\|_{TV}\,\rho_r^M(d\nu)\le c_{\mathsf{Ent}}.$$

Hence, we can conclude

$$S_\ell(t)\le S_\ell(0)+c_{\mathsf{Ent}}t$$

Hence, since $\mathsf{Ent}(\rho_0^M|\hat\Pi^k)<\infty$, we can conclude by the dominated convergence theorem that

$$\mathsf{Ent}(\rho_t^M|\hat\Pi^k)\le \mathsf{Ent}(\rho_0^M|\hat\Pi^k)+c_{\mathsf{Ent}}t.$$

□

5.3 Compactness result

In Chapter 4, we proved the existence and uniqueness of global solutions to the truncated forward Kolmogorov equation (4.1.1). However, there we looked at a truncated version of adjoint operator L^*. We want to extend these results to establish existence of a solution to the original problem. As a tool to extend these results, we consider weak solutions for this problem.

Definition 5.3.1. Recall $\rho := (\rho_t)_{t\ge 0}\in C([0,T],\mathcal{M}^+(\hat\Gamma_X))$ is a weak solution to the forward Kolmogorov equation with initial data $\rho_0=\bar\rho$ if it satisfies

$$\langle F,\rho_t\rangle-\langle F,\rho_s\rangle=\int_s^t\langle LF,\rho_r\rangle\,dr \qquad \forall\,F\in C_b(\hat\Gamma_X),\ (s,t)\subset[0,T]. \tag{5.3.1}$$

We want to prove that a solution to equation (5.3.1) exists. The idea is to consider a sequence $(\rho_t^M)_{M\in\mathbb{N}}$ where for every $M\in\mathbb{N}$, $\rho_t^M=u_t^M d\hat\Pi^k$ with u_t^M a solution to the truncated forward Kolmogorov equation (4.1.1). We assume $\int_{\hat\Gamma_X}u_0(\nu)d\hat\Pi^k=1$ and know this solution exists and is unique due to Theorem 4.1.4. Therefore, for every $M\in\mathbb{N}$, this ρ_t^M satisfies

$$\langle F,\rho_t^M\rangle-\langle F,\rho_s^M\rangle=\int_s^t\langle L^MF,\rho_r^M\rangle\,dr \qquad \forall\,F\in C_b(\hat\Gamma_X),\ (s,t)\subset[0,T] \tag{5.3.2}$$

Our goal now is to show $\{(\rho_t^M)_{t\ge0}\}_{M\in\mathbb{N}}$ has a convergent subsequence, which implies the existence of a solution to (5.3.1).

The main result of this chapter is given in the following theorem.

Theorem 5.3.2. *Let operator L be given by (2.3.2), where the rates satisfy Assumption 2.3.4. Let X be a compact subset of a separable metric space, with $\lambda(X) \leq \infty$. Then there exists a solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T]; \mathcal{M}^+(\hat{\Gamma}_X))$ to problem (5.3.1).*

The proof of this Theorem requires several steps. We want to prove there exists a weak solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T]; \mathcal{M}^+(\Gamma_X))$ first. Note, that we consider the configuration space Γ_X as defined in (5.1.1), rather than $\hat{\Gamma}_X$. The reason for this is that we want to apply a refined version of Ascoli-Arzelà's Theorem as in [1] and the conditions are easier to check for Γ_X. Therefore, we begin the proof of Theorem 5.3.2 by proving that the conditions of Ascoli-Arzelà's Theorem are satisfied. Hence, let $\rho_t^M(\nu)$ be a solution to weak problem (5.3.2) with L_M^* as defined in (4.1.2). Then the first three steps consist of proving the following.

A1) Γ_X is a separable metric space. (Lemma 5.3.3)

A2) There exists a K such that $\rho_t^M \subset K$ for all $t \in [0,T]$ where K is relatively compact in Γ_X with respect to the narrow topology. (Proposition 5.3.4)

A3) $\{(\rho_t^M)_{t\geq 0}\}_{M\in\mathbb{N}}$ is equicontinuous with respect to the total variation norm. (Lemma 5.3.5)

Once we proved this, we use a refined version of Ascoli-Arzelà's Theorem to prove

A4) The sequence $\{(\rho_t^M)_{t\geq 0}\}_{M\in\mathbb{N}}$ has a convergent subsequence in $\mathcal{M}^+(\Gamma_X)$. (Theorem 5.3.6)

When we established this subsequence exists, we know that for this subsequence, the left-hand side of (5.3.2) converges to the left-hand side of (5.3.1). We want to establish convergence of the right-hand side as well. Hence, we want to prove that

A5) For this subsequence, it holds that

$$\lim_{M\to\infty} \int_s^t \langle L^M F, \rho_r^M \rangle \, dr = \int_s^t \langle LF, \rho_r \rangle \, dr. \quad \text{(Theorem 5.4.1)}$$

Once, we have proved this, we can prove there exists a solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T]; \mathcal{M}^+(\Gamma_X))$ to problem (5.3.1). However, we require a solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T]; \mathcal{M}^+(\hat{\Gamma}_X))$. We note that $\hat{\Gamma}_X \subset \Gamma_X$ and we demand $\rho_0 \in \mathcal{M}^+(\hat{\Gamma}_X)$. Therefore, we want to prove that if ρ is a solution to (5.3.1) with $\rho_0 \in \mathcal{M}^+(\hat{\Gamma}_X)$, this implies $\rho_t \in \mathcal{M}^+(\hat{\Gamma}_X)$ for all $t \in [0,T]$. Hence, we want to show

A6) If a solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T]; \mathcal{M}^+(\Gamma_X))$ is a solution to (5.3.1) with initial data given by $\rho_0 \in \mathcal{M}^+(\hat{\Gamma}_X)$ then $\rho_t \in \mathcal{M}^+(\hat{\Gamma}_X)$ for all $t \in [0,T]$. (Theorem 5.4.2)

Once we have proved this, we can conclude Theorem 5.3.2 holds. We even have that this solution is absolutely continuous, so we end this chapter by proving the following

A7) The solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T]; \mathcal{M}^+(\hat{\Gamma}_X))$ is absolutely continuous. (Lemma 5.4.3)

We start by proving Property A1)

Lemma 5.3.3. Let X be a compact subset of a separable metric space. Then Γ_X is a separable metric space.

Proof. We consider Γ_X endowed with the total variation norm. We have to prove that Γ_X is separable with respect to the this norm.
Since X is separable, there exists a countable set Y such that $\overline{Y} = X$. This means the set $[\bigsqcup_{n=0}^\infty Y^n]^k$ is also countable.
Let $\nu \in \Gamma_X$. Then $\nu = (\sum_{i=1}^{n_1} \delta_{x_i}, \ldots, \sum_{i=1}^{n_k} \delta_{x_i})$. For each x_i, there exists a sequence $(y_i^\ell)_{\ell\in\mathbb{N}} \in Y$ such that $y_i^\ell \to x_i$.

Let $\nu^\ell = (\sum_{i=1}^{n_1} \delta_{x_i^\ell}, \dots, \sum_{i=1}^{n_k} \delta_{x_i^\ell})$. We want to show $\nu^\ell \to \nu$ in the total variation norm. This result follows from simple computations if we can prove that $y^\ell \to x$ implies $\delta_{y^\ell} \to \delta_x$ in total variation norm. We have that

$$\left\| \int_X g(z) d\delta_x(z) - \int_X g(z) d\delta_{y^\ell}(z) \right\| = \left\| g(x) - g(y^\ell) \right\|.$$

$\left\| g(x) - g(y^\ell) \right\| \to 0$ for all $g \in C_0(X)$, $\|g\| \le 1$ if $y^\ell \to x$. Hence, $\left\| \delta_x - \delta_{y^\ell} \right\|_{TV} \to 0$. □

From Lemma 5.1.1, we find that the sequence $\{(\rho_t^M)_{t\ge 0}\}_{M\in\mathbb{N}}$ defined as before satisfies

$$\rho_t^M \in K := \left\{ \rho \in \mathcal{P}(\Gamma_X) : \int_{\Gamma_X} \|\nu\|_{TV} \, \rho(d\nu) \le c_1 \right\} \qquad \text{for all } t \in [0,T] \text{ and } M \in \mathbb{N},$$

with c_1 given by (5.1.2).

Proposition 5.3.4. *The set K defined above is relatively compact w.r.t. the narrow topology.*

Proof. We prove the set K is tight and apply Prokhorov's Theorem [1]. To show tightness, we define the set

$$K_N := \left\{ \nu \in \Gamma_X : \|\nu\|_{TV} \le N \right\} \subset \Gamma_X.$$

This set is narrowly compact in Γ_X. By the Markov inequality, we find

$$\int_{\Gamma_X \setminus K_N} \rho_t^M(d\nu) \le \int_{\Gamma_X} \frac{\|\nu\|_{TV}}{N} \rho_t^M(d\nu) \le \frac{c_1}{N}.$$

c_1 is the constant given by (5.1.2). Tightness of the set K follows by taking the limit $N \to \infty$. Therefore, by Prokhorov's Theorem K is relatively compact. □

Lemma 5.3.5. Let $T > 0$ and let $(\rho_t^M)_{M\in\mathbb{N}} : [0,T] \to \Gamma_X$ with $\rho_t^M \in K$ for all $M \in \mathbb{N}$ and $t \in [0,T]$ where K is a σ-relatively compact set in Γ_X. Then $\{(\rho_t^M)_{t\ge 0}\}_{M\in\mathbb{N}}$ is equicontinuous with respect to the total variation norm.

Proof. This result follows from Lemma 5.1.1, since

$$\left\| \rho_t^M - \rho_s^M \right\|_{TV} = \sup_{\|F\|_{\sup} \le 1} |\langle F, \rho_t^M \rangle - \langle F, \rho_s^M \rangle| \le c_1 C_L |t-s|$$

Therefore, we can conclude the set $\{(\rho_t^M)_{t\ge 0}\}_{M\in\mathbb{N}}$ is equicontinuous with respect to the total variation norm. □

Theorem 5.3.6. *The sequence $\{(\rho_t^M)_{t\ge 0}\}_{M\in\mathbb{N}}$ has a convergent subsequence in $\mathcal{M}^+(\Gamma_X)$.*

Proof. The theorem follows directly from Lemma 5.3.4 and Lemma 5.3.5 and the application of Proposition 3.3.1 (A refined version of Ascoli-Arzelà theorem) from [1]. □

5.4 Existence weak solution

In Theorem 5.3.6, we proved the existence of a convergent subsequence. However, before we can conclude there exists a solution to (5.3.1), we must ensure that we can pass to the limit in (5.3.2). The following Theorem ensures that we can do this at least in Γ_X.

Theorem 5.4.1. *Let $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\Gamma_X))$ and let $\{(\rho_t^M)_{t\geq 0}\}_{M\in\mathbb{N}}$ be a subsequence (not relabelled) such that*

$$\rho_t^M \rightharpoonup \rho_t \qquad \text{for all } t \in [0,T],$$

where $\rightharpoonup$ denotes narrow convergence and let

$$\langle F, \rho_t^M\rangle \to \langle F, \rho_t\rangle \qquad \text{for all } F \in C_b(\Gamma_X).$$

Then

$$\lim_{M\to\infty} \int_s^t \langle L^M F, \rho_r^M\rangle \, dr = \int_s^t \langle LF, \rho_r\rangle \, dr.$$

Proof. We want to use the Generalized Dominated Convergence Theorem. We note that

$$|L^M F(\nu)| \leq C_L \|F\|_{\sup} \|\nu\|_{TV}.$$

This means our claim follows if we can prove

$$\lim_{M\to\infty} \int_{\Gamma_X} \|\nu\|_{TV} \, \rho_r^M(d\nu) = \int_{\Gamma_X} \|\nu\|_{TV} \, \rho_r(d\nu).$$

We have for all $n \in \mathbb{N}$

$$\begin{aligned}\lim_{M\to\infty} \int_{\Gamma_X} \|\nu\|_{TV} \, \rho_r^M(d\nu) &= \lim_{M\to\infty} \left(\int_{\|\nu\|_{TV}\leq n} \|\nu\|_{TV} \, \rho_r^M(d\nu) + \int_{\|\nu\|_{TV}>n} \|\nu\|_{TV} \, \rho_r^M(d\nu) \right), \\ &= \int_{\|\nu\|_{TV}\leq n} \|\nu\|_{TV} \, \rho_r(d\nu) + \lim_{M\to\infty} \int_{\|\nu\|_{TV}>n} \|\nu\|_{TV} \, \rho_r^M(d\nu).\end{aligned}$$

We then have

$$\begin{aligned}\lim_{M\to\infty} \int_{\|\nu\|_{TV}>n} \|\nu\|_{TV} \, \rho_r^M(d\nu) &\leq \lim_{M\to\infty} \int_{\Gamma_X} \frac{\|\nu\|_{TV}^2}{n} \rho_r^M(d\nu), \\ &\leq \lim_{M\to\infty} \frac{c_2}{n} = \frac{c_2}{n}.\end{aligned}$$

Here, c_2 is given by (5.1.5). Hence, we have

$$\int_{\|\nu\|_{TV}\leq n} \|\nu\|_{TV} \, \rho_r(d\nu) \leq \lim_{M\to\infty} \int_{\Gamma_X} \|\nu\|_{TV} \, \rho_r^M(d\nu) \leq \int_{\|\nu\|_{TV}\leq n} \|\nu\|_{TV} \, \rho_r(d\nu) + \frac{c_2}{n}.$$

The claim follows by letting $n \to \infty$. □

At this moment, we used Ascoli-Arzelà to prove there exists $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\Gamma_X))$ and a subsequence (not relabelled) such that

$$\rho_t^M \rightharpoonup \rho_t \qquad \text{for all } t \in [0,T].$$

To uphold our modeling assumptions, however, we require a solution with $\rho_t \in \mathcal{M}^+(\hat{\Gamma}_X)$, $\forall t \in [0,T]$. First of all, we note that $\mathcal{M}^+(\hat{\Gamma}_X) \subset \mathcal{M}^+(\Gamma_X)$. Furthermore, we note that $\rho_0 = \bar{\rho} \in \mathcal{M}^+(\hat{\Gamma}_X)$. Therefore, we know that if $\bar{\rho} \in \mathcal{M}^+(\hat{\Gamma}_X)$ implies $\rho_t \in \mathcal{M}^+(\hat{\Gamma}_X)$ for all $t \in [0,T]$ then we found our required solution $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\hat{\Gamma}_X))$.

Theorem 5.4.2. *Let $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\Gamma_X))$ be a solution to (5.3.1) with initial data $\rho_0 = \bar{\rho} \in \mathcal{M}^+(\hat{\Gamma}_X)$ then $\rho_t \in \mathcal{M}^+(\hat{\Gamma}_X)$ for all $t \in [0,T]$.*

Proof. Since $\rho_t^M \rightharpoonup \rho_t$ narrowly, for all $t \in [0,T]$, it holds that

$$\mathsf{Ent}(\rho_t|\hat{\Pi}^k) \leq \liminf_{M\to\infty} \mathsf{Ent}(\rho_t^M|\hat{\Pi}^k) \leq \mathsf{Ent}(\rho_0|\hat{\Pi}^k) + c_{\mathsf{Ent}} t.$$

Hence, we know $\mathsf{Ent}(\rho_t|\hat{\Pi}^k)$ is bounded. Therefore, by definition, we know that ρ_t is absolutely continous with respect to $\hat{\Pi}^k$. Since $\hat{\Pi}^k(\nu) = 0$ for $\nu \notin \hat{\Gamma}_X$, we conclude $\rho_t \in \mathcal{M}^+(\hat{\Gamma}_X)$ for all $t \in [0,T]$. □

Proof of Theorem 5.3.2. Lemma 5.3.6 gives the existence in of a solution $(\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\Gamma_X))$. The weak problem (5.3.1) requires $\rho_0 \in \mathcal{M}^+(\hat{\Gamma}_X)$. Therefore by application of Theorem 5.4.2, it holds that $(\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\hat{\Gamma}_X))$. □

Lemma 5.4.3. Suppose $\rho = (\rho_t)_{t\in[0,T]} \in C([0,T];\mathcal{M}^+(\hat{\Gamma}_X))$ is a solution to weak problem (5.3.1). Then this solution is absolutely continuous in the total variation norm.

Proof. According to Lemma 5.1.1, we have for all $M \in \mathbb{N}$ and all $t, s \in [0,T]$

$$|\langle F, \rho_t^M\rangle - \langle F, \rho_s^M\rangle| \leq c_1 C_L \|F\|_{\sup}|t-s|.$$

Since this bound is independent of M, we can conclude

$$\limsup_{M\in\mathbb{N}} \sup_{F\in C_c(\Gamma_X),\|F\|\leq 1} |\langle F, \rho_t^M\rangle - \langle F, \rho_s^M\rangle| \leq \sup_{F\in C_c(\Gamma_X),\|F\|\leq 1} c_1 C_L \|F\|_{\sup}|t-s| \leq c_1 C_L|t-s|.$$

In Lemma 5.3.4, tightness was established. Therefore, the absolute continuity follows. □

Chapter 6

Scaling and mean field limit

6.1 Mean field limit

In this chapter, we aim to scale our interacting particle system and derive the mean field limit. In other words, we want to look at a measure $\bar{\nu} = (\bar{\nu}_1, \ldots, \bar{\nu}_k)$ satisfying equations of the form

$$\partial_t \bar{\nu}_m = V_m(\bar{\nu}) \tag{6.1.1}$$

for all $m \in \{1, \ldots, k\}$.

In this chapter, we consider $X := \mathbb{Z}^d \cap \Omega$, where Ω is compact. We assume all transitions can occur but do not consider births and deaths in this system. Nonetheless, we do note that in X the number of particles is always finite. Therefore, we could consider "empty particles" as a specific type of particle as well. If a particle transitions from an empty type to a particle of type i, this could be seen as "birth" of type i even though on the level of the generator we considered this as a transition. The reason we could not do this before is because we only assumed compactness of X and therefore could not guarantee the finiteness of the number of particles.

Moreover, we make an additional assumption on the rates. This assumption is

Assumption 6.1.1. The rate functions κ_{ij} have the following form for all $i, j \in \{1, \ldots, k\}, i \neq j$,

$$\kappa_{ij}(x, \nu) = \psi_{ij}\left(\sum_{\ell=1}^{M} \int_X \phi_{ij}^{\ell}(x, y)\nu_\ell(dy)\right) \qquad \text{for } x \in X \text{ and } \nu \in \hat{\Gamma}_X.$$

Here, we assume ψ_{ij} is continuous and locally Lipschitz and $\phi_{ij}^{\ell} \in L^\infty(X^2)$ for all $\ell \in \{1, \ldots, M\}$. Moreover, $\nu_\ell(dy) = \lambda(dy)\mathbb{1}_{y \in \text{supp } \nu_\ell}$.

The idea behind the mean field limit is to scale the grid as $X_N := \frac{1}{N}\mathbb{Z}^d \cap \Omega$, for $N \in \mathbb{N}$, and let N go to infinity. The result leads to a system of integro-differential equations for the measure $\bar{\nu}$. First, we explain the scaling itself and then we derive the limit.

The scaling of the grid affects several aspects of our model. We begin with the scaling of the intensity measure λ. For any $N \geq 1$, set

$$\lambda_N = \sum_{x \in X_N} \delta_x \in \mathcal{M}^+(\Omega). \tag{6.1.2}$$

Since the number of points in X_N grows when N grows, we expect the mass of this intensity measure to increase as well. We rescale the map $\Lambda^{n,k}$ given by (2.4.2) to counterbalance this growth. For any $A \subset \Omega$ with $\text{dist}(A, \partial\Omega) > 1/2N$, we find that

$$\lambda_N(A) = \#\{x \in X^N \cap A\} = N^d |A^N|, \qquad A^N = \bigcup_{x \in X^N \cap A} Q_{\frac{1}{2N}}(x),$$

where $Q_r(x)$ is the cube of radius $r > 0$ around $x \in \Omega$. Furthermore, $|A_N|$ denotes the Lebesgue measure of A_N. Hence, the intensity $\lambda^N(A)$ of a set A grows as N^d, suggesting to rescale the map $\Lambda^{n,k}$, $n = n_1 + \cdots + n_k$, as

$$\Lambda_N^{n,k} : X_N^{n_1} \times \cdots \times X_N^{n_k} \to \Gamma_\Omega := [\mathcal{M}^+(\Omega)]^k;$$
$$((x_1^1, \ldots, x_{n_1}^1), \ldots, (x_1^k, \ldots, x_{n_k}^k)) \mapsto \left(\frac{1}{N^d} \sum_{i=1}^{n_1} \delta_{x_i^1}, \ldots, \frac{1}{N^d} \sum_{i=1}^{n_k} \delta_{x_i^k} \right).$$

Consequently, the rescaled Lebesgue-Poisson measure reads

$$\lambda_N^\infty = \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{1}{\prod_{p=1}^k n_p!} \lambda_N^{\otimes n_1} \otimes \cdots \otimes \lambda_N^{\otimes n_k}, \tag{6.1.3}$$

and $\Pi_N^k = (\Lambda_N^{n,k})_\# \lambda_N^\infty$ is the scaled counterpart for $\hat{\Pi}^k$ defined in (2.4.3). The next step is to consider the rate functions. Let $\kappa_{ij}(x,\nu)$ satisfy Assumption 6.1.1 and let $\phi_{ij}^{\ell,N} := N^{-d} \phi_{ij}^\ell$ then

$$\begin{aligned} \kappa_{ij}(x,\nu) &= \psi_{ij} \left(\sum_{\ell=1}^M \int_X \phi_{ij}^\ell(x,y) \nu_\ell(dy) \right) = \psi_{ij} \left(\sum_{\ell=1}^M N^d \int_X \phi_{ij}^{\ell,N}(x,y) \nu_\ell(dy) \right) \\ &= \psi_{ij} \left(\sum_{\ell=1}^M \sum_{y \in \nu_\ell} \phi_{ij}^{\ell,N}(x,y) \right) =: \kappa_{ij}^N(x,\nu) \end{aligned}$$

These scaled rates are necessary to define the scaled generator. Since we only consider transitions in this model, we can write the generator as

$$L^N F(\nu) = \sum_{i,j \neq i} \sum_{x \in \nu_i} \left[F\left(\nu - \frac{1}{N^d} \delta_x e_i + \frac{1}{N^d} \delta_x e_j \right) - F(\nu) \right] \kappa_{ij}^N(x,\nu).$$

The factors $\frac{1}{N^d}$ in the argument of the test function F, are a result of the scaling as well. This first argument expresses the configuration after a particular transitioning. Since this transition now happens on the grid X^N, it follows that this expression should be scaled as well. Moreover, it holds that

$$\begin{aligned} L^N F(\nu) &= \sum_{i,j \neq i} \sum_{x \in \nu_i} \left[F\left(\nu - \frac{1}{N^d} \delta_x e_i + \frac{1}{N^d} \delta_x e_j \right) - F(\nu) \right] \kappa_{ij}^N(x,\nu) \\ &= \sum_{i,j \neq i} N^d \int_X \left[F\left(\nu - \frac{1}{N^d} \delta_x e_i + \frac{1}{N^d} \delta_x e_j \right) - F(\nu) \right] \kappa_{ij}(x,\nu)\, \nu_i(dx). \end{aligned}$$

We want to know what happens when we let N go to infinity. To investigate this, we consider the scaled generator for a specific type of test functions: cylindrical functions.

A cylindrical function is a function of the form

$$F(\nu) = f\big((\langle g_1^1, \nu_1 \rangle, \ldots \langle g_{m_1}^1, \nu_1 \rangle), \ldots, (\langle g_1^k, \nu_k \rangle, \ldots \langle g_{m_k}^k, \nu_k \rangle) \big),$$

where f is continuously differentiable and g is continuous and bounded.

For any cylindrical function, we have that

$$\lim_{N \to \infty} N^d \left[F\left(\nu - \frac{1}{N^d} \delta_x e_i + \frac{1}{N^d} \delta_x e_j \right) - F(\nu) \right] = -D_i f \cdot g^i(x) + D_j f \cdot g^j(x).$$

This equality follows from the linear approximation of $F\left(\nu - \frac{1}{N^d}\delta_x e_i + \frac{1}{N^d}\delta_x e_j\right)$. Due to linearity of the function F most terms vanish when subtracting $F(\nu)$, leaving terms depending on i and j.

When we consider the generator and note that we can interchange limit and integral since X is compact, we obtain for any $\nu \in \hat{\Gamma}_X$

$$\widehat{L}F(\nu) := \lim_{N\to\infty} L^N F(\nu) = \sum_{i,j\neq i} \int_X \left[-D_i f \cdot g^i(x) + D_j f \cdot g^j(x)\right] \kappa_{ij}(x,\nu)\, \nu_i(dx).$$

Now let ρ^N be a weak solution of the scaled problem

$$\langle F, \rho_t^N\rangle - \langle F, \rho_s^N\rangle = \int_s^t \int_{\Gamma_\Omega} L^N F(\nu)\, \rho_r^N(d\nu)\, dr. \tag{6.1.4}$$

Suppose that

$$\rho_t^N \rightharpoonup \hat{\rho}_t \qquad \text{narrowly in } \hat{\Gamma}_X \text{ for every } t \in [0,T].$$

If we take the limit of both sides of (6.1.4) and use that we can interchange integral and limit again, we find for any cylindrical function F, $\hat{\rho}$ satisfies

$$\langle F, \hat{\rho}_t\rangle - \langle F, \hat{\rho}_s\rangle = \int_s^t \int_{\Gamma_\Omega} \widehat{L}F(\nu)\, \hat{\rho}_r(d\nu)\, dr. \tag{6.1.5}$$

We say that a curve $t \mapsto \hat{\rho}_t$ is a weak solution of the Liouville equation $\partial_t \rho_t = \widehat{L}^* \rho_t$ if (6.1.5) holds for all cylindrical functions and all $[s,t] \subset [0,T]$.

Eventually, we are interested in finding a system of integro-differential equations, which is only possible if $\hat{\rho}_t$ concentrates. With this in mind, we motivate a candidate weak solution to the Liouville equation in the following. Suppose for the moment that $\hat{\rho}_t = \delta_{\hat{\nu}_t}$ for some curve $t \mapsto \hat{\nu}_t$. Then

$$\frac{d}{dt}\langle F, \hat{\rho}_t\rangle = \frac{d}{dt} F(\hat{\nu}_t) = \sum_{i=1}^k D_i f \cdot \langle g^i, \partial_t \hat{\nu}_i\rangle.$$

On the other hand,

$$\begin{aligned}\widehat{L}F(\hat{\nu}) &= \sum_{i,j\neq i} \int_X \left[-D_i f \cdot g^i(x) + D_j f \cdot g^j(x)\right] \psi_{ij} \left(\sum_{\ell=1}^M \int_\Omega \phi_{ij}^\ell(x,y)\, \hat{\nu}_\ell(dy)\right) \hat{\nu}_i(dx) \\ &= \sum_{i=1}^k D_i f \cdot \left\langle g^i, -\left(\sum_j \kappa_{ij}(\cdot,\hat{\nu})\right)\hat{\nu}_i + \left(\sum_j \kappa_{ji}(\cdot,\hat{\nu})\hat{\nu}_j\right)\right\rangle.\end{aligned}$$

This second equality follows from an index switch of dummy variable i and j.

Therefore, if $\hat{\nu}$ satisfies

$$\partial_t \hat{\nu}_i = -\left(\sum_j \kappa_{ij}(\cdot,\hat{\nu})\right)\hat{\nu}_i + \left(\sum_j \kappa_{ji}(\cdot,\hat{\nu})\hat{\nu}_j\right) =: V_i(\hat{\nu}), \qquad i = 1,\dots,k, \tag{6.1.6}$$

then the curve $t \mapsto \hat{\rho}_t = \delta_{\hat{\nu}_t}$ is a weak solution of the Liouville equation.

6.2 Well-posedness

We want to prove system (6.1.6) is well-posed. We define operator A as

$$A\bar{\nu} := -\left(\sum_j \psi_{ij}\left(\int \phi_{ij} d\bar{\nu}_j\right)\right) d\bar{\nu}_i + \left(\sum_j \psi_{ji}\left(\int \phi_{ji} d\bar{\nu}_i\right) d\bar{\nu}_j\right) \tag{6.2.1}$$

Lemma 6.2.1. Under Assumption 6.1.1, operator $A : [\mathcal{M}(\Omega)]^k \to [\mathcal{M}(\Omega)]^k$ is Lipschitz continuous in the total variation norm.

Proof. We only prove Lipschitz continuity for the first term for arbitrary i and j. The proof for the second term works analogously. We have

$$\begin{aligned}
&\sup_{\|\varphi\|_{\sup}\le 1} \left\{ -\int \varphi\psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\nu}_\ell \right) d\bar{\nu}_i + \int \varphi\psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\omega}_\ell \right) d\bar{\omega}_i \right\} \\
&= \sup_{\|\varphi\|_{\sup}\le 1} \left\{ -\int \varphi\psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\nu}_\ell \right) d\bar{\nu}_i + \int \varphi\psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\omega}_\ell \right) (d\bar{\omega}_i - d\bar{\nu}_i + d\bar{\nu}_i) \right\}, \\
&= \sup_{\|\varphi\|_{\sup}\le 1} \left\{ \int \varphi \left(\psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\omega}_\ell \right) - \psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\nu}_\ell \right) \right) d\bar{\nu}_i + \int \varphi\psi_{ij} \left(\sum_{\ell=1}^{M} \int \phi_{ij}^{\ell} d\bar{\omega}_\ell \right) (d\bar{\omega}_i - d\bar{\nu}_i) \right\}, \\
&\le \sup_{\|\varphi\|_{\sup}\le 1} \left\{ \int \varphi \left(\overline{\psi_{ij}} \sum_{\ell=1}^{M} \left| \int \phi_{ij}^{\ell} d\bar{\omega}_\ell - \int \phi_{ij}^{\ell} d\bar{\nu}_\ell \right| \right) d\bar{\nu}_i + \int \varphi \overline{\psi_{ij}} \sum_{\ell=1}^{M} \left| \int \phi_{ij}^{\ell} d\bar{\omega}_\ell \, (d\bar{\omega}_i - d\bar{\nu}_i) \right| \right\}, \\
&\le \sum_{\ell=1}^{M} \overline{\psi_{ij}} \left\| \phi_{ij}^{\ell} \right\|_{L^\infty} \|\bar{\nu}_i\|_{TV} \|\bar{\omega}_\ell - \bar{\nu}_\ell\|_{TV} + \overline{\psi_{ij}} \left\| \phi_{ij}^{\ell} \right\|_{L^\infty} \|\bar{\omega}_\ell\|_{TV} \|\bar{\omega}_i - \bar{\nu}_i\|_{TV} .
\end{aligned}$$

Here, $\overline{\psi_{ij}}$ is the locally Lipschitz constant that exists due to our assumptions. □

We define the Lipschitz constant of operator A as L_A.

Lemma 6.2.2. Under Assumpion 6.1.1, the system of differential equations (6.1.5) has a unique solution.

Proof. Let $A : [\mathcal{M}(\Omega)]^k \to [\mathcal{M}(\Omega)]^k$ and let $\bar{\omega} \in C([0,\infty); [\mathcal{M}(\Omega)]^k)$. We define an operator $B : C([0,\infty); [\mathcal{M}(\Omega)]^k) \to C([0,\infty); [\mathcal{M}(\Omega)]^k)$ as

$$B\bar{\omega}(t) = \bar{\omega}(0) + \int_0^t A\bar{\omega}(s)ds. \tag{6.2.2}$$

Furthermore, we define the following norm on the space $C([0,\infty); [\mathcal{M}(\Omega)]^k)$

$$|||\bar{\omega}|||_\lambda := \sup_{t\in[0,\infty)} \left(\|\bar{\omega}(t)\|_{TV} \, e^{-\lambda t} \right)$$

Then we have for $\bar{\nu}$ and $\bar{\omega}$ with $\bar{\nu}(0) = \bar{\omega}(0)$, that

$$\begin{aligned}
|||B\bar{\nu}(t) - B\bar{\omega}(t)|||_\lambda &= \sup_{t\geq 0} e^{-\lambda t} \left\| \bar{\nu}(0) + \int_0^t A\bar{\nu}(s)ds - \bar{\nu}(0) - \int_0^t A\bar{\omega}(s)ds \right\|_{TV}, \\
&\leq \sup_{t\geq 0} e^{-\lambda t} \int_0^t \|A\bar{\nu}(s) - A\bar{\omega}(s)\|_{TV} \, ds, \\
&\leq L_A \sup_{t\geq 0} e^{-\lambda t} \int_0^t \|\bar{\nu}(s) - \bar{\omega}(s)\|_{TV} \, ds, \\
&\leq L_A \sup_{t\geq 0} e^{-\lambda t} \int_0^t e^{\lambda s} e^{-\lambda s} \|\bar{\nu}(s) - \bar{\omega}(s)\|_{TV} \, ds, \\
&\leq L_A |||\bar{\nu} - \bar{\omega}|||_\lambda \sup_{t\geq 0} e^{-\lambda t} \int_0^t e^{\lambda s} ds, \\
&= L_A |||\bar{\nu} - \bar{\omega}|||_\lambda \sup_{t\geq 0} \frac{1}{\lambda}(1 - e^{-\lambda t}), \\
&\leq \frac{L_A}{\lambda} |||\bar{\nu} - \bar{\omega}|||_\lambda.
\end{aligned}$$

We choose $\lambda = L_A + 1$. Then the operator B is a contraction with respect to norm $|||\cdot|||_\lambda$. Hence, by Banach Fixed point Theorem operator B has a unique fixed point which is a unique global solution to (6.1.5). □

In this chapter, we derived a mean field limit for a general type of interacting particle systems with rate functions satisfying Assumptions 2.3.4 and 6.1.1. Moreover, we established well-posedness for the limiting system of integro-differential equations. In the next chapter, we look at an application of these results to a tumor growth model.

Chapter 7

Application to tumor growth model

7.1 Tumor growth model

In the remainder of this report, we consider a specific type of interacting particle system. We use the theory on interacting particles to formulate a tumor growth model. The goal is to investigate the mean field limit we found in Chapter 6 for this specific application. First, we investigate a two-dimensional tumor growth model. We want to compare the solution of the system of integro-differential equations with both the original stochastic simulation of this interacting particle system as well as two scaled versions of this stochastic simulation. Since the computations for a two-dimensional model become too large, we also investigate a one-dimensional model. First, however, we explain the model and give a biological background to justify the considered cell types.

The model in this report is based on the model in [7]. We consider four different types of cells: healthy, proliferative, non-proliferative and necrotic cells. The healthy cells are the only cells not part of the tumor. We explain the different parts of the tumor next. Formally, we can define proliferative cells as follows:

Definition 7.1.1. *Proliferative cells* are cells with the ability to grow and increase in number rapidly [2].

When a tumor starts growing, it consists of proliferative cells only. Proliferative cells are tumor cells that are able to divide, where division of cells requires space. We assume the proliferative cells close to the tumor boundary always have enough space, being able to push the healthy cells aside. In terms of the interacting particles, we say healthy cells transition to proliferative cells. At some point in time, however, the tumor becomes so large that inner tumor cells are too far from the boundary and consequently the required space is unavailable. If these cells are still alive, they are called non-proliferative. Formally, the definition is given by:

Definition 7.1.2. The *non-proliferative cells* are cells that do not divide but retain the ability the re-enter cell proliferation [12].

When the tumor grows even larger at some point the inner core turns necrotic.

Definition 7.1.3. *Necrotic cells* are cells that died uncontrollably before the end of the cells' natural life span [11].

Intuitively, necrotic cells can be seen as dead cells in the core of the tumor. Nutrients necessary for cells survival cannot reach the inner core anymore leading to the death of these cells. Since these dead cells cannot disappear, they still require space and are therefore not negligible. Figure 7.1 illustrates this model. White cells are the healthy cells, red forms the proliferative layer, green the non-proliferative layer and black the necrotic core. This image is two-dimensional and can be viewed as a cross section of the tumor. The one-dimensional model we consider later can be seen as the diameter of this cross section and still gives a representation of tumor growth if we assume spherical symmetry.

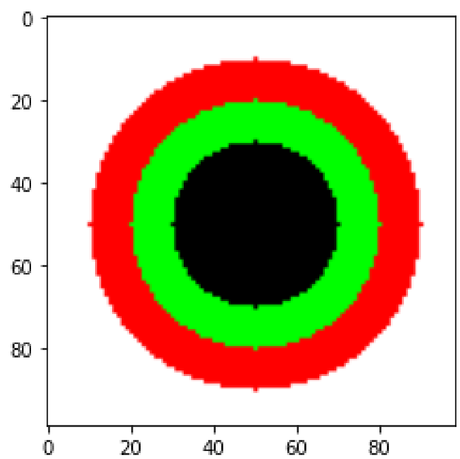


Figure 7.1: Tumor growth model

In our two-dimensional model, the tumor is modelled as a Markov process on grid X, where $X := \mathbb{Z}^2 \cap \Omega$, with Ω a compact set. The grid points represent the centers of the tumor cells. We give these points values to represent their state. We consider four different state values given by the set $\{0, 1, 2, 3\}$. The zeros denote the healthy cells. The $\{1, 2, 3\}$ stand for the proliferative, non-proliferative and necrotic cells, respectively. Due to the discrete nature of the tumor cells and the Markov property of the process, we view this process as an interacting particle system. In particular, this model is an example of the contact process [10]. Due to the compactness of Ω and since we consider $\mathbb{Z}^2$, we can conclude that the number of cells are always finite. This is the case since $|\Omega|$ is finite and each cell has uniformly positive measure. Hence, we can consider 0-particles as their own type. We call these particles the 0-type particles to emphasize the fact that they are not part of the tumor. This leads to a slight abuse of notation, because we consider e_0 as the unit normal vector belonging to the zero-particles. This can be regarded as e_4 in this example. We note that we formulated the mean field limit in the previous chapter for particles starting with index 1, but this is just a matter of notation.

In this tumor growth model the following transitions can occur:

(i) Particles of type 0 can transition to type 1.

(ii) Particles of type 1 can transition to type 0 and type 2.

(iii) Particles of type 2 can transition to type 1 and type 3.

First, we note that only transitions occur. This is because we include 0-type particles in our specification of types rather than considering them as empty. This is due to the compactness of Ω, resulting in a finite number of 0-particles. From a biological reasoning, we want the rates to satisfy the following properties:

(i) The transition rate of a 0-particle at position x increases if the number of 1-particles in a neighbourhood of x increases.

(ii) The transition rate of a 1-particle to a 0-particle at position x increases if the number of 0-particles in a neighbourhood of x increases.

(iii) The transition rate of a 1-particle to a 2-particle at position x increases if the number of 0-particles in a neighbourhood of x decreases.

(iv) The transition rate of a 2-particle to a 1-particle at position x increases if the number of 0-particle in a neighbourhood of x increases.

(v) The transition rate of a 2-particle to a 3-particle at position x increases if the number of 0-particles and the number of 1-particles in a neighbourhood of x decreases.

The generator of this model has the form

$$LF(\nu) = \sum_{i,j \neq i} \sum_{x \in \nu_i} \left[F\left(\nu - \delta_x e_i + \delta_x e_j\right) - F(\nu) \right] \kappa_{ij}(x, \nu).$$

We consider the following transition rates:

1. For the transitioning of an empty cell to a proliferative cell, we define the following rate function: $\kappa_{01}(y,\nu) := c_{01} \int \mathbb{1}_{\{z \in X : |z-x|_{\ell^\infty} \leq 1\}}(y)\, \nu_1(dx) \mathbb{1}_{\nu_0}(y)$.
Heuristically, this is counting the proliferative neighbours of the empty cell, multiplied by some constant $c_{01} \in \mathbb{R}_0^+$.

2. A proliferative cell at position y can turn healthy with rate: $\kappa_{10}(y,\nu) := c_{10} \int \mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y) \nu_0(dx) \mathbb{1}_{\nu_1}(y)$.

3. A proliferative cell at position x can turn non-proliferative with rate: $\kappa_{12}(y,\nu) := c_{12}(e^{-\int \mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y)\, \nu_0(dx)} - e^{-|\mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y)|}) \mathbb{1}_{\nu_1}(y)$.

4. A non-proliferative cell at position y can turn proliferative with rate: $\kappa_{21}(y,\nu) := c_{21} \int \mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y) \nu_0(dx) \mathbb{1}_{\nu_2}(y)$.

5. A non-proliferative cell at position x can turn necrotic with rate: $\kappa_{23}(y,\nu) := c_{23}(e^{-\int \mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y)\, \nu_0(dx) - \int \mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y) \nu_1(dx)} - e^{-|\mathbb{1}_{z \in X : |z-x|_{\ell^\infty} \leq 1}(y)|}) \mathbb{1}_{\nu_2}(y)$.

For all the other possible transitions, we say $\kappa_{ij}(y,\nu) = 0$. We note that we can write the rates above in the form $\kappa_{ij} = \psi_{ij}\left(\sum_{\ell=1}^{M} \int_X \phi_{ij}^{\ell}(x,y)\nu_\ell(dy)\right)$, where ψ_{ij} is continuous and locally Lipschitz and ϕ_{ij}^{ℓ} is bounded. ψ_{01}, ψ_{10} and ψ_{21} are now just identity functions for these specific rates.

Based on the theory derived in the previous chapter, we find that the mean field limit of this interacting particle system is given by (6.1.6).

In the next section, we are going to investigate the solution to system (6.1.6) for this tumor growth model and compare this solution with three stochastic simulations of the interacting particle system. One of these simulations is the original interacting particle system and the other two are scaled versions of this system.

7.2 Simulation

In this section, we compare four different numerical simulations. The first is the numerical solution of integro-differential system (6.1.5) for the tumor growth model. The second simulation is the original interacting particle system, the third is a scaled version where $N = 2$ and the fourth is a scaled version where $N = 4$. In the original system, we consider a grid of 100 by 100 and the scaling leads to a grid of $N \cdot 100$ by $N \cdot 100$. Since the integro-differential system is the limit found after scaling, we expect that the scaled versions of the interacting particle system are closer to the solution of the integro-differential equations than the original model.

Since the interacting particle system is stochastic, we want to take the average over a number of runs in both scaled and the original systems. This average is taken by running the simulation several times and determining for each cell and each time step the number of times that cell is healthy, proliferative, non-proliferative and necrotic. This number is then divided by the number of runs. This means we find for each cell and each time step fractions of the different particle types. The fraction belonging to a certain particle type, for example the proliferative type, suggest how frequently a specific cell was proliferative on average at a specific time. The closer this number is to 1, the more likely it is that the cell is proliferative at the considered time. The idea behind this stochastic simulation is summarized in Algorithm 1.

Algorithm 1 Pseudocode interacting particle system

procedure STOCHASTIC SIMULATION
    Initialize grid and set count to 0
    Calculate the rate of all the possible transitions in every cell
    Sum all the rates
    Draw random exponential with rate equal to the sum
    Add exponential to count
    Choose which transition occurs at random proportional to the total sum of all the possible transitions
    Choose which cell transitions at random proportional to the rates of the cells with respect to the chosen transitioning
    Repeat until count > 200

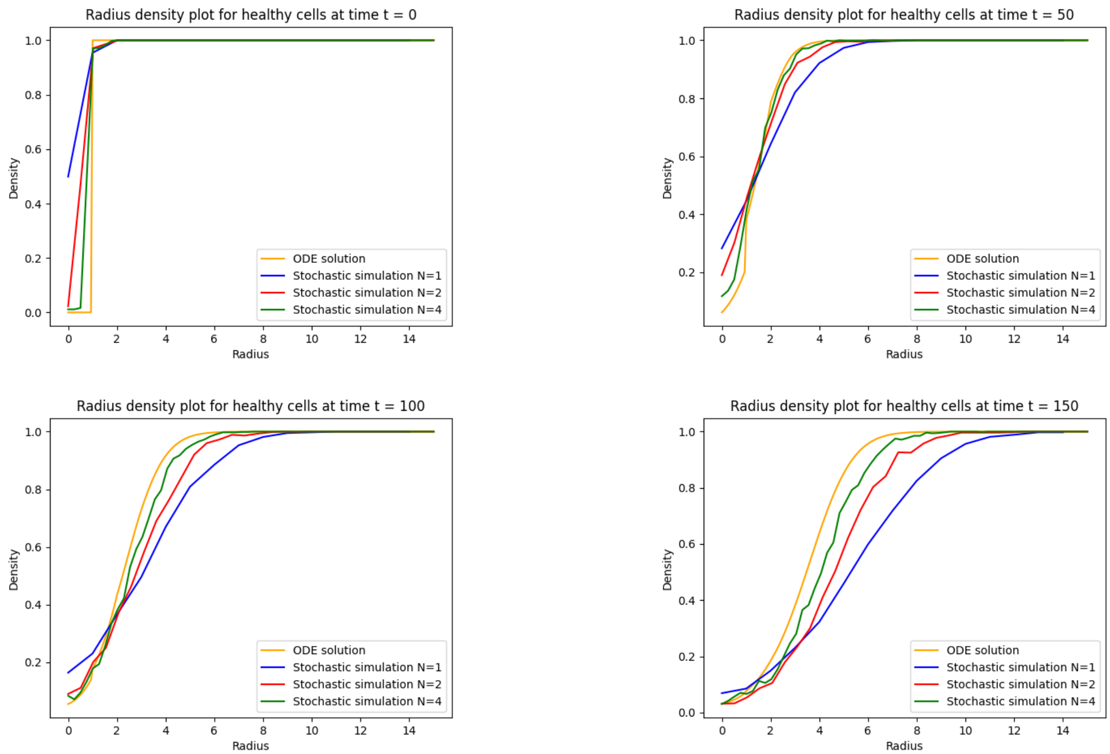
For the simulation of the solution of the integro-differential equations, we discretize our grid. Since this solution is the limit after scaling the grid size, we want the grid size to be much smaller than the grid sizes in all the stochastic simulations. For the solution of the ODE, we scaled the grid with a factor 15. For a higher scaling factor, the computations become too demanding. The simulation of the solution of the system of integro-differential equations is summarized in Algorithm 2.

Algorithm 2 Pseudocode ODE solution

procedure SIMULATION ODE SOLUTION
    Initialize grid
    Formulate solution as large vector $(\bar{\nu}_0, \bar{\nu}_1, \bar{\nu}_2, \bar{\nu}_3)$
    Formulate system of integro-differential equations in a vector form
    Solve by using ODE solver

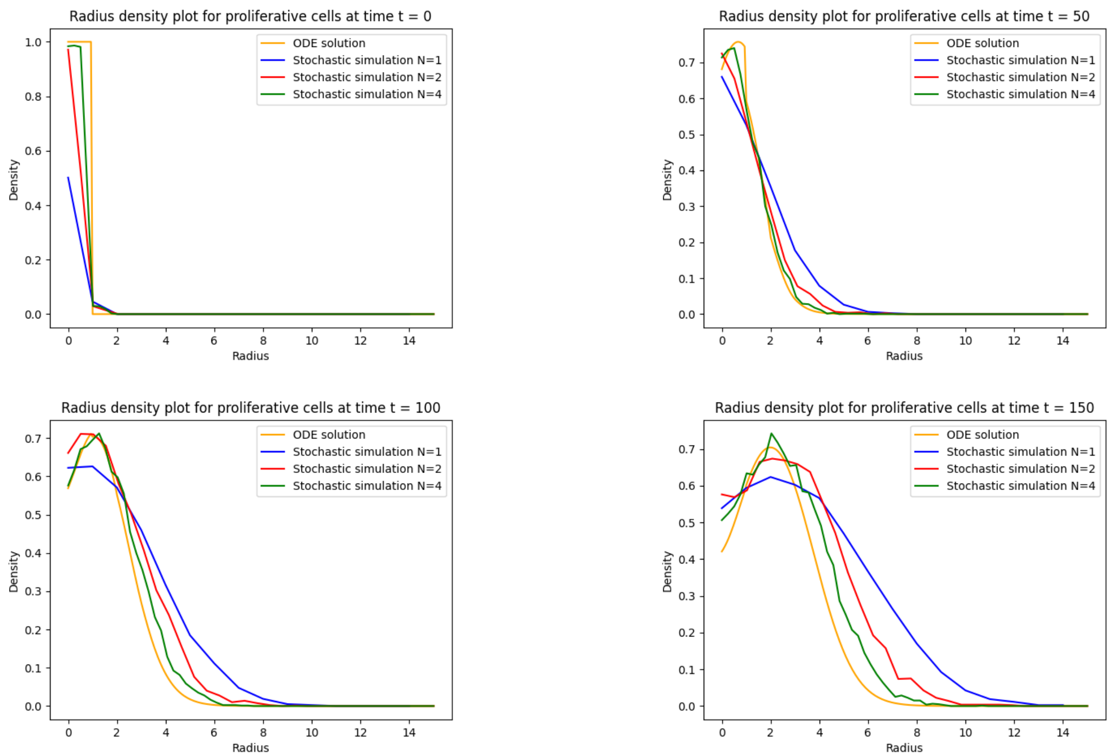
The solution of the system of integro-differential equations also gives numbers between zero and one. Therefore, this solution and the stochastic simulations are easy to compare. We start by comparing with a radius-density plot. Due to the spherical symmetry of the tumor, we can investigate the densities of the tumor along the radius. We can do the same for the two averaged scaled and the original interacting particle systems. The solutions of these three simulation are approximately spherically symmetric if the number of runs we use to average is large enough. To improve the plot, we also average along the radii in four different directions. We find the following results.

Figure 7.2: Radius-density plots for the healthy cells of the ODE solution, normal simulation and scaled simulation



For the healthy cells, we notice that the radius-density plots for the normal stochastic simulation, both the scaled stochastic simulations and the ODE solution are relatively close. This is a promising result since it means our microscopic and macroscopic model describe the same phenomenon. We notice that the stochastic simulation for $N = 4$ is closest to the ODE solution, whereas $N = 2$ is the second best match. This is in line with what we expect. Furthermore, the difference between the original simulation and the scaled simulation with $N = 2$ seems to be larger than the difference between the two different scaled simulations. This is also promising since this suggests convergence to the ODE solution. We do note, however, that the size of the grid in the discretization for the determination of the ODE solution is equivalent to a scaling of the grid size with $N = 15$. Since we want to investigate the limiting behaviour, it would be more interesting to simulate the ODE solution for a finer grid. However, this system becomes too large to solve.

Figure 7.3: Radius-density plots for the proliferative cells of the ODE solution, normal simulation and scaled simulation



For the proliferative cells, we can again conclude that the four models are relatively close to each other. Again, the higher the scaling factor N, the closer the graph is to the graph of the ODE solution. In both the comparison of the non-proliferative cells and the necrotic cells, which are given in Figure 7.4 and 7.5 the convergence of the stochastic simulations to the ODE solution is also clear.

Figure 7.4: Radius-density plots for the non-proliferative cells of the ODE solution, normal simulation and scaled simulation

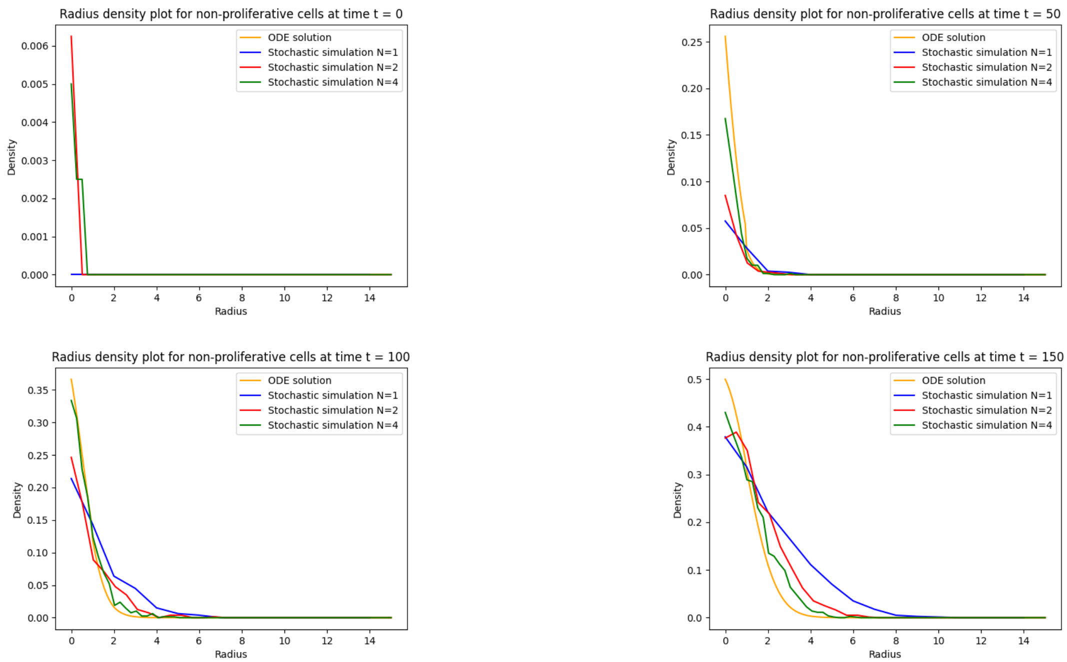
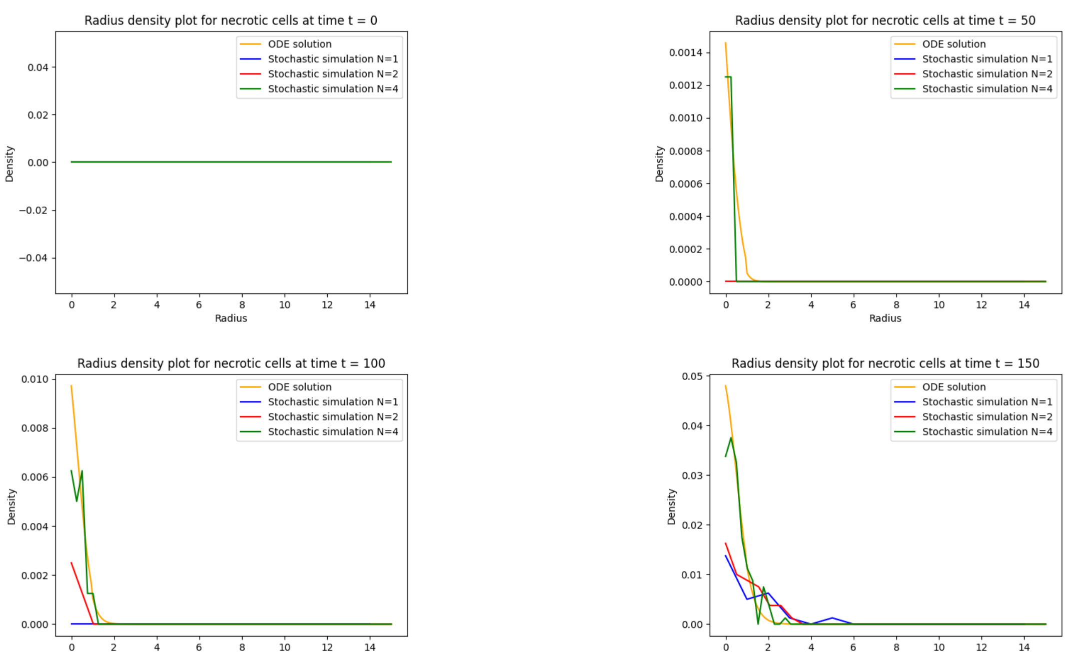
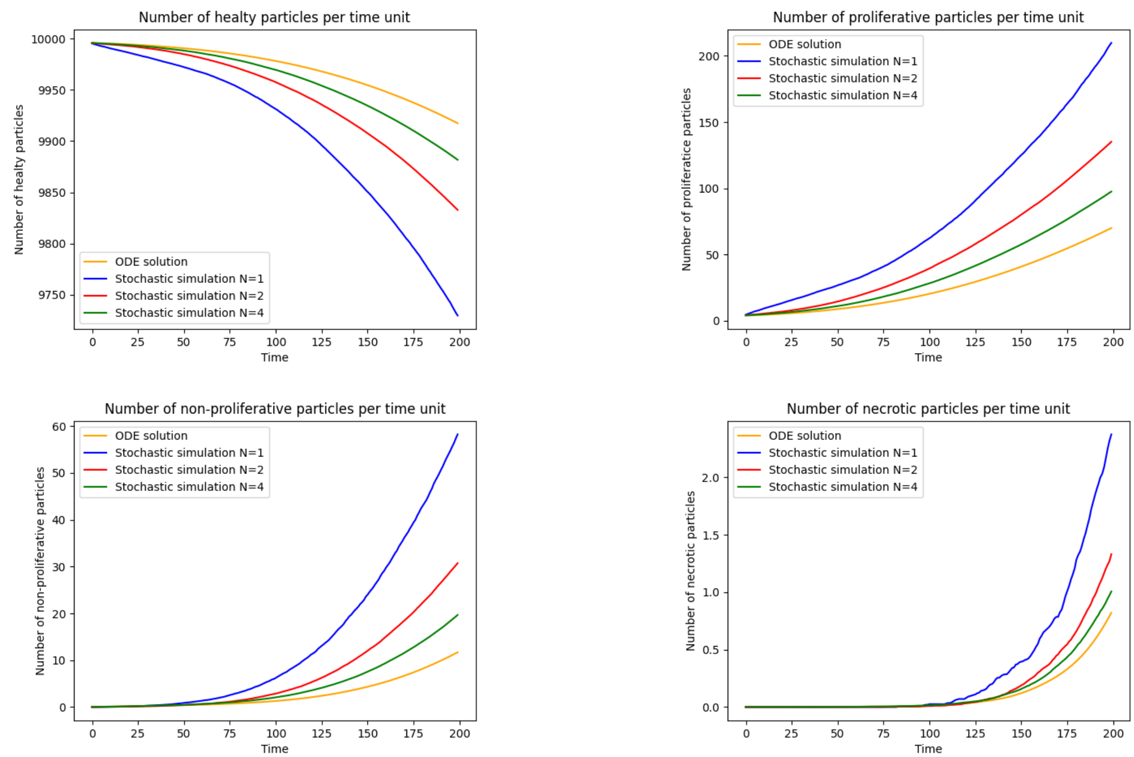


Figure 7.5: Radius-density plots for the necrotic cells of the ODE solution, normal simulation and scaled simulation



For further comparison, we calculate the average number of healthy, proliferative, non-proliferative and necrotic cells. Furthermore, we normalize such that these values are in between 0 and 10000 as in the original interacting particle system. This way we can compare these values. These graphs are displayed in Figure 7.6

Figure 7.6: Number of different type of particles per time unit



Again, we notice that the scaled stochastic simulation for $N = 4$ is closest to the ODE solution. Likewise, the stochastic simulation with $N = 2$ is the second best fit. Moreover, the difference between the original interacting particle system and the simulation with $N = 2$ seems to be larger than the difference between the stochastic simulations with $N = 2$ and $N = 4$. This suggests convergence of the scaled stochastic simulations to the ODE solution which is precisely what we would expect.

In the next figures, we plot the spread of healthy cells, proliferative cells and non-proliferative cells for several times. We do not plot the necrotic cells since the number of necrotic cells is too small to be interesting.

Figure 7.7: Spread of healthy cells in ODE solution and stochastic simulations for t = 50

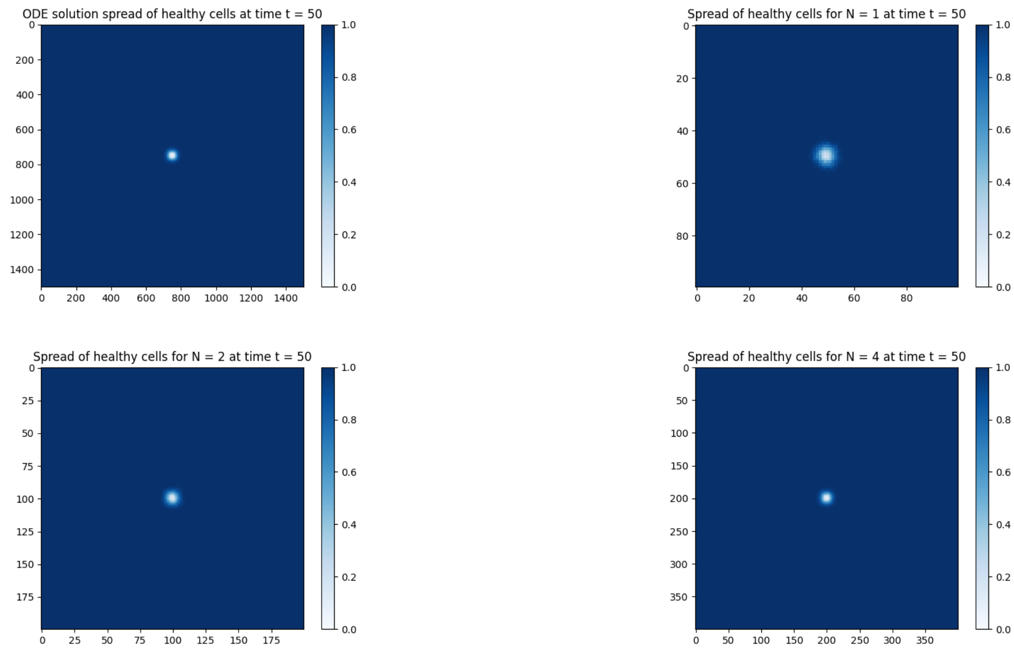


Figure 7.8: Spread of healthy cells in ODE solution and stochastic simulations for t = 100

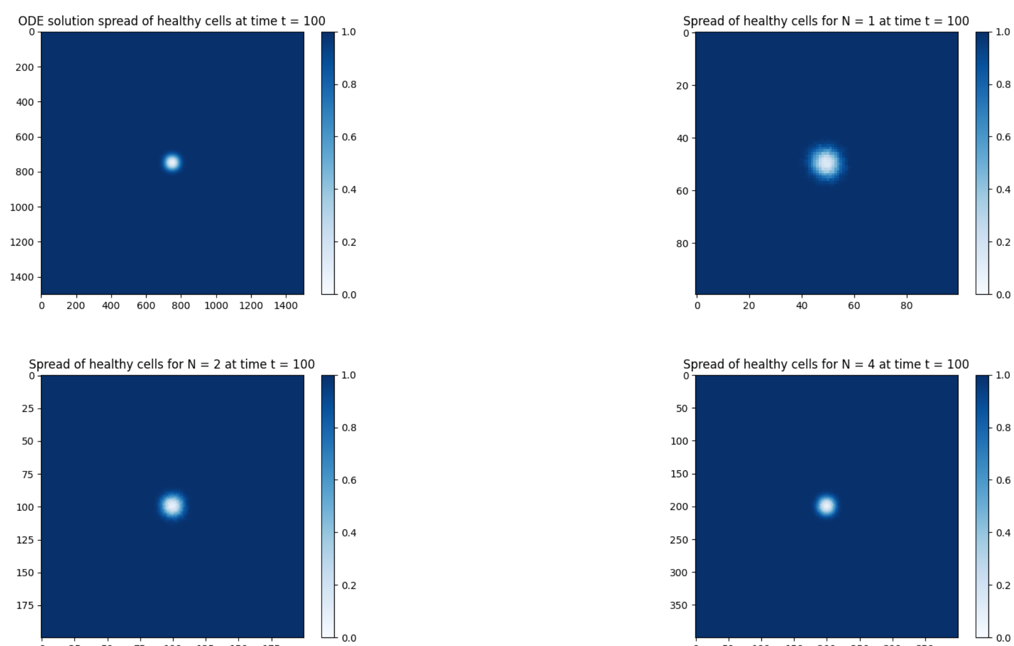


Figure 7.9: Spread of healthy cells in ODE solution and stochastic simulations for t = 150

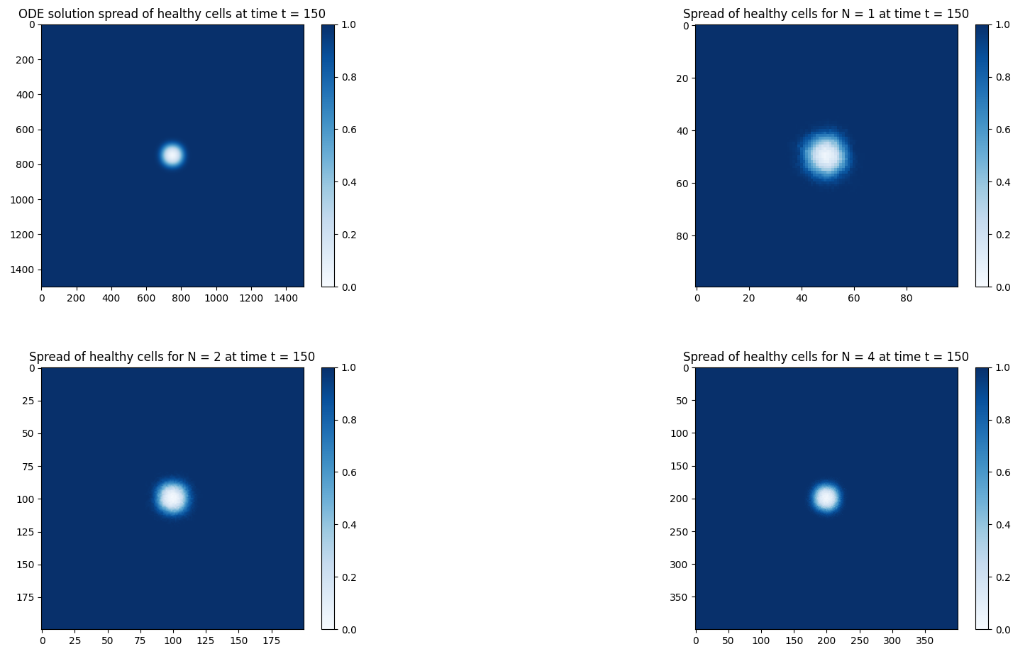


Figure 7.10: Spread of proliferative cells in ODE solution and stochastic simulations for t = 50

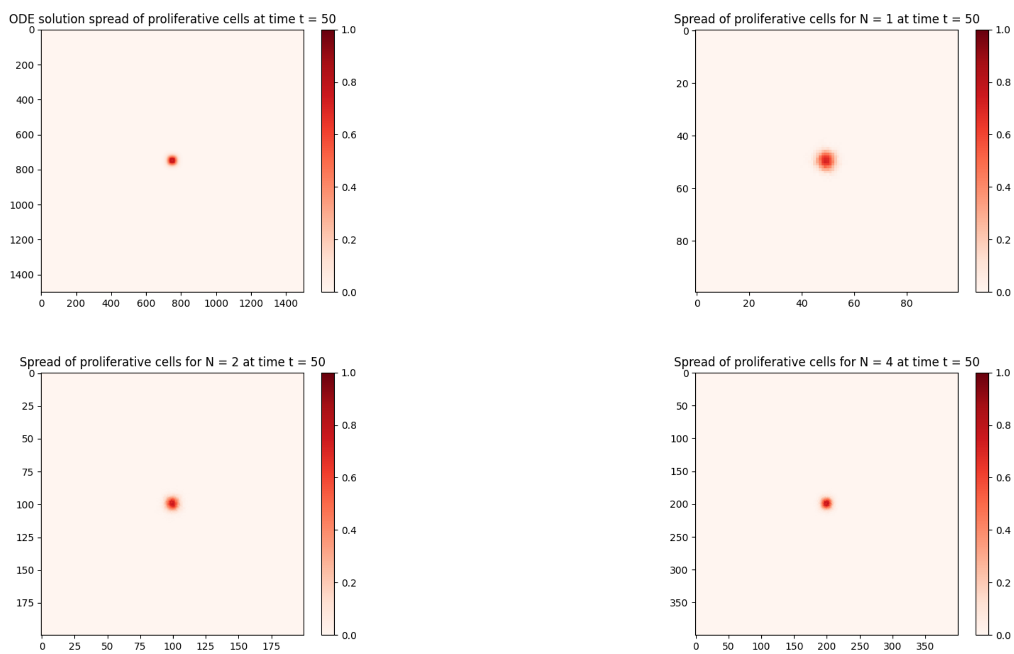


Figure 7.11: Spread of proliferative cells in ODE solution and stochastic simulations for t = 100

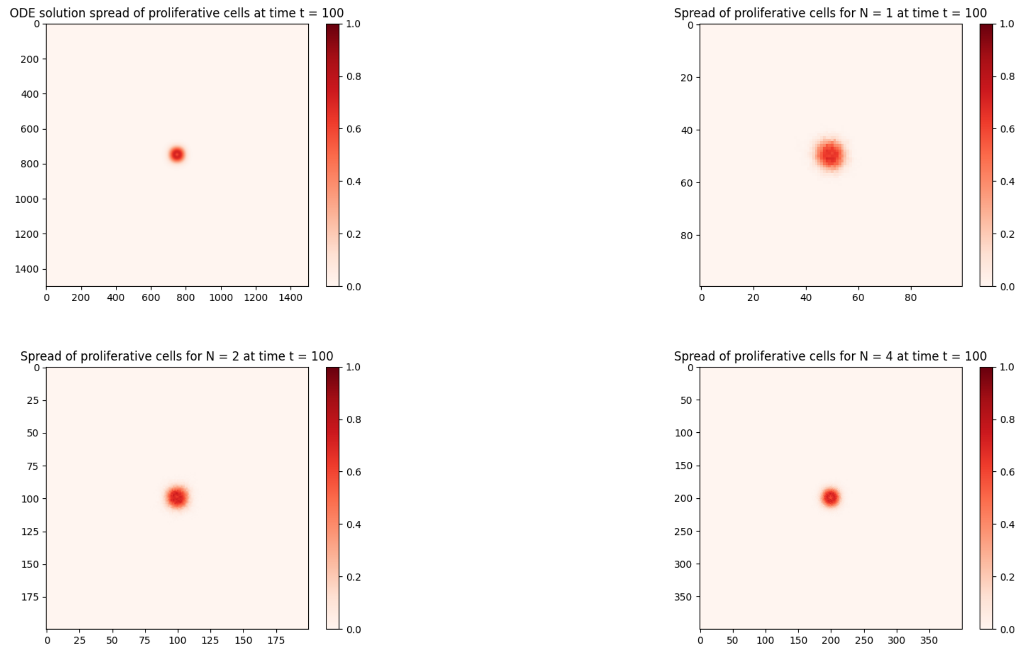


Figure 7.12: Spread of proliferative cells in ODE solution and stochastic simulations for t = 150

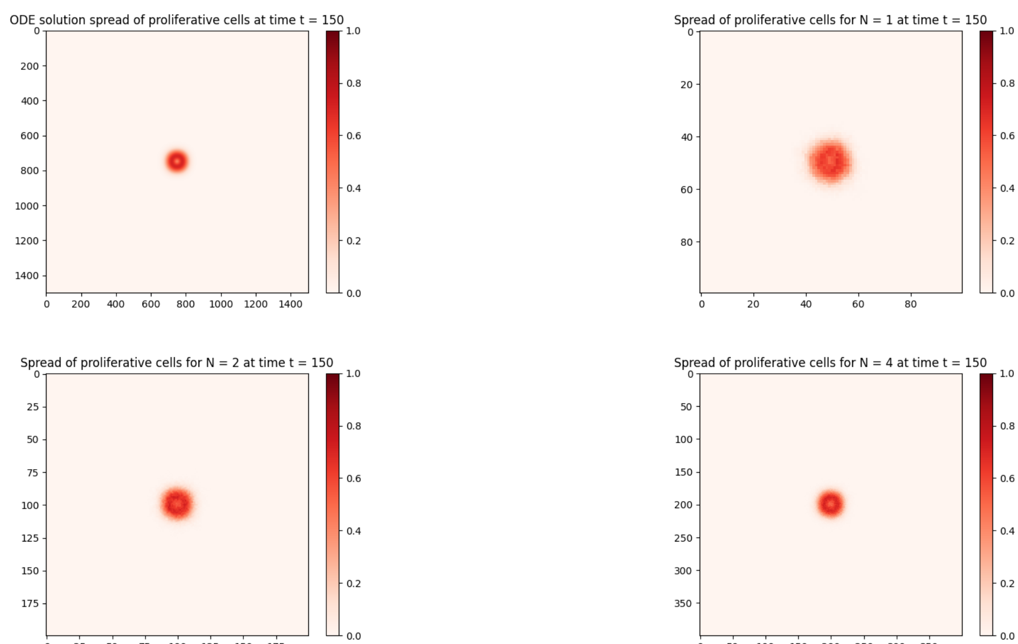


Figure 7.13: Spread of non-proliferative cells in ODE solution and stochastic simulations for t = 50

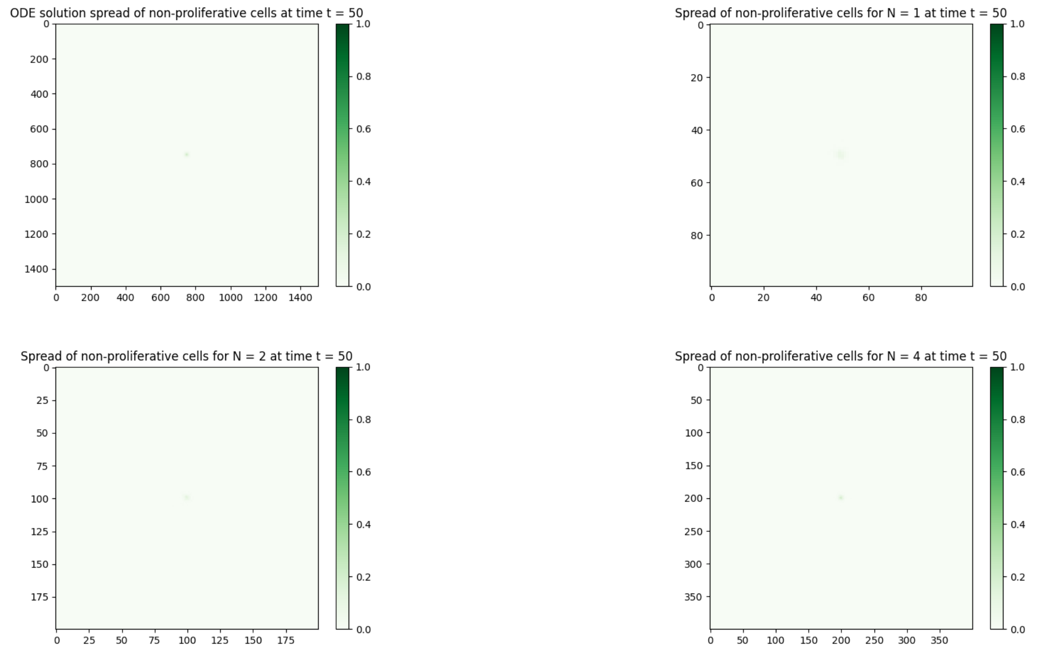


Figure 7.14: Spread of non-proliferative cells in ODE solution and stochastic simulations for t = 100

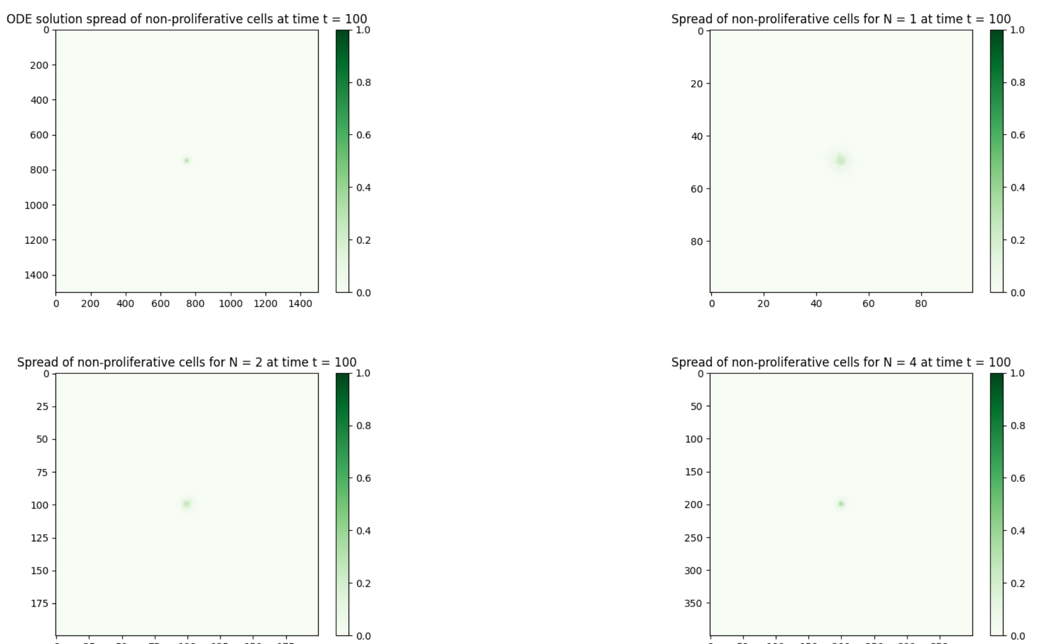
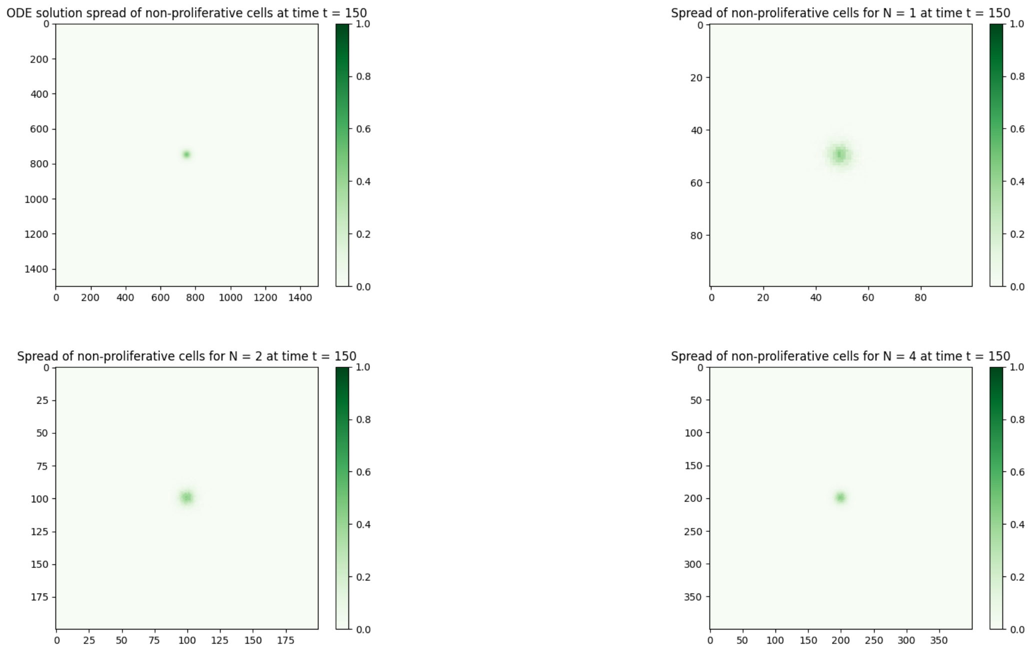


Figure 7.15: Spread of non-proliferative cells in ODE solution and stochastic simulations for t=150



To conclude, we find a converging trend of the scaled interacting particle systems towards the ODE solution. This is promising, because it is precisely what we expect to see based on the calculations of the mean field limit.

As we mentioned before, however, we want to consider a finer grid in the discretization used to simulate the ODE solution. The discretization we want to consider is equivalent to a grid after scaling with $N = 1000$. In practice, however, the computations in this case are too demanding. Every grid point leads to four differential equations because we have four types of particles. This leads to a system with $4 \cdot (N \cdot 100)^2$ number of differential equations which is too large to solve. Therefore, we consider a one-dimensional simulation in the next section. This decrease of dimension also leads to a major decrease of the number of differential equations which enables us to investigate a discretization equivalent to a grid after scaling with a factor $N = 1000$.

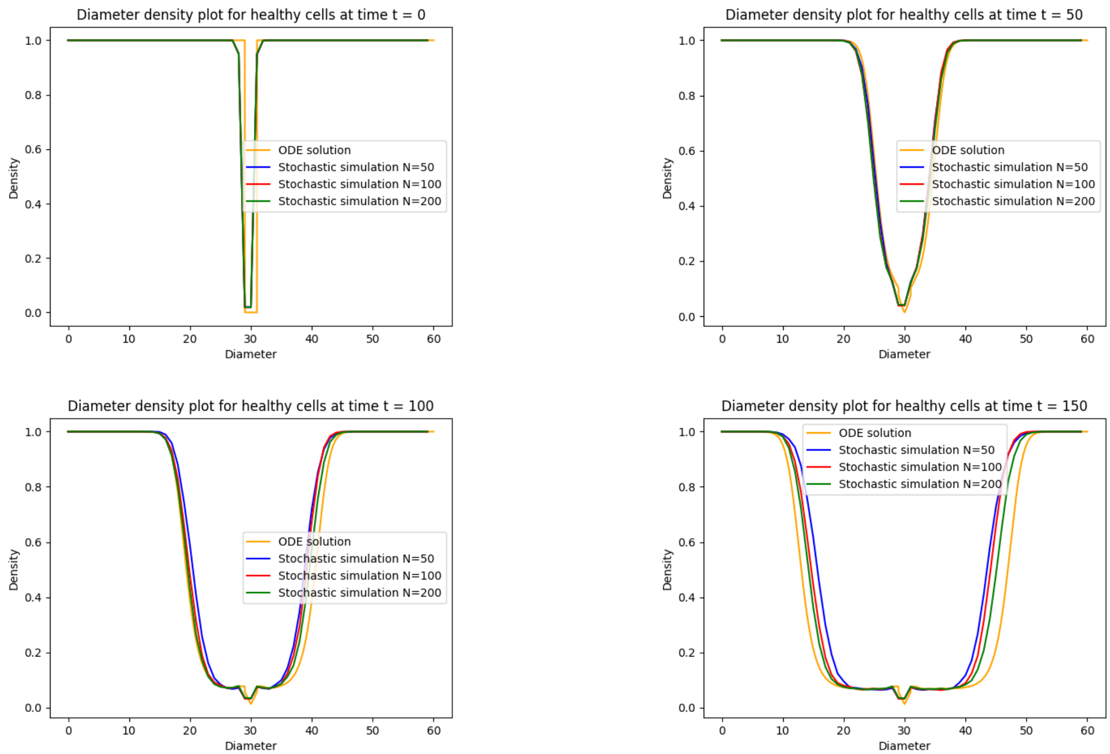
7.3 One-dimensional simulation

As mentioned before, we want to check whether the simulations of the scaled interacting particle system converge to the solution of the system of integro-differential equations. To simulate the solution of the integro-differential equation by means of an ODEsolver in Python, discretization of our state space is required. However, since the grid size in the scaled versions of the interacting particle systems decreases, and the solution of the integro-differential equations is the limit found after letting the grid size converge to zero, we want the discretization steps to be much smaller than the grid size in the interacting particle systems. In the two-dimensional case this leads to a problem due to too demanding computations. Therefore, a one-dimensional interacting particle system is investigated.

In this one-dimensional model, we consider again healthy, proliferative, non-proliferative and necrotic cells. The rate functions are also similar to the rate functions considered for the two-dimensional model, although the rate constants are altered to find more interesting results.

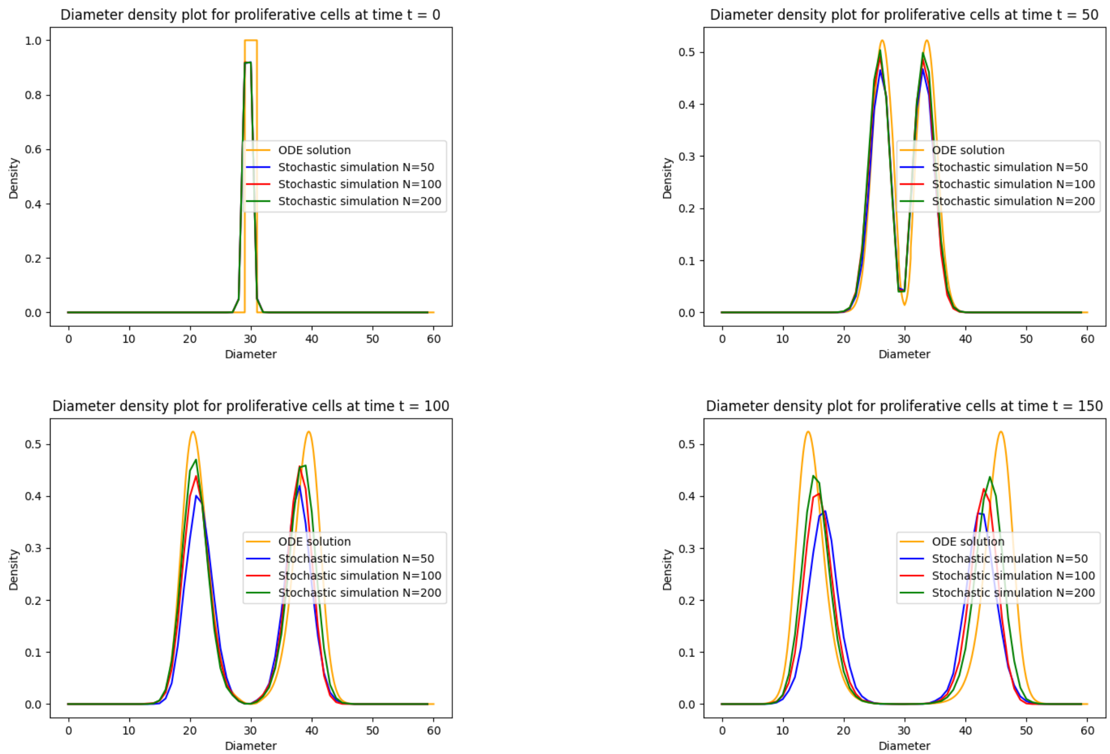
We display the density at every point in the interval of our one-dimensional interacting particle system. If we assume spherical symmetry, these densities can be regarded as the diameter of the tumor.

Figure 7.16: Diameter-density plots for the healthy cells of the ODE solution, normal simulation and scaled simulations



We were able to determine the ODE solution in a grid discretized in a way equivalent to scaling with $N = 1000$. For smaller times, lines are all very close. However, for $t = 100$, we notice that the stochastic simulation for $N = 200$ is closest to the ODE solution. This becomes clearer for $t = 150$. It is clear that the larger N is, the better the interacting particle system resembles the ODE solution. This seems to be an additional confirmation the mean field limit is correct.

Figure 7.17: Diameter-density plots for proliferative cells of the ODE solution, normal simulation and scaled simulations



In the diameter-density plots for the proliferative cells, we notice a similar result as for the healthy cells. If we increase N the fit between the stochastic simulation and the ODE solution becomes better. We notice for $t = 100$ and $t = 150$ that there is still some distance between the lines of the stochastic simulations and the ODE solution, but a converging trend is visible. In Figure 7.18 and Figure 7.19, we display the diameter-density plots for the non-proliferative cells and necrotic cells, respectively. We again see a converging trend, where the stochastic simulation becomes closer to the solution of the ODE solution for higher N.

Figure 7.18: Diameter-density plots for non-proliferative cells of the ODE solution, normal simulation and scaled simulations

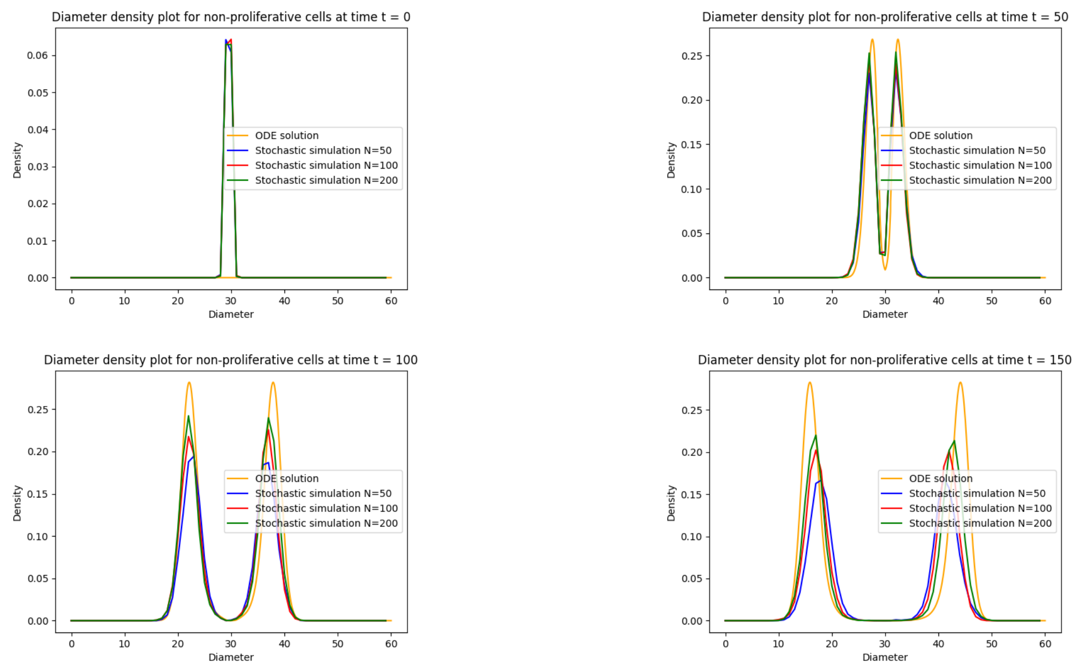
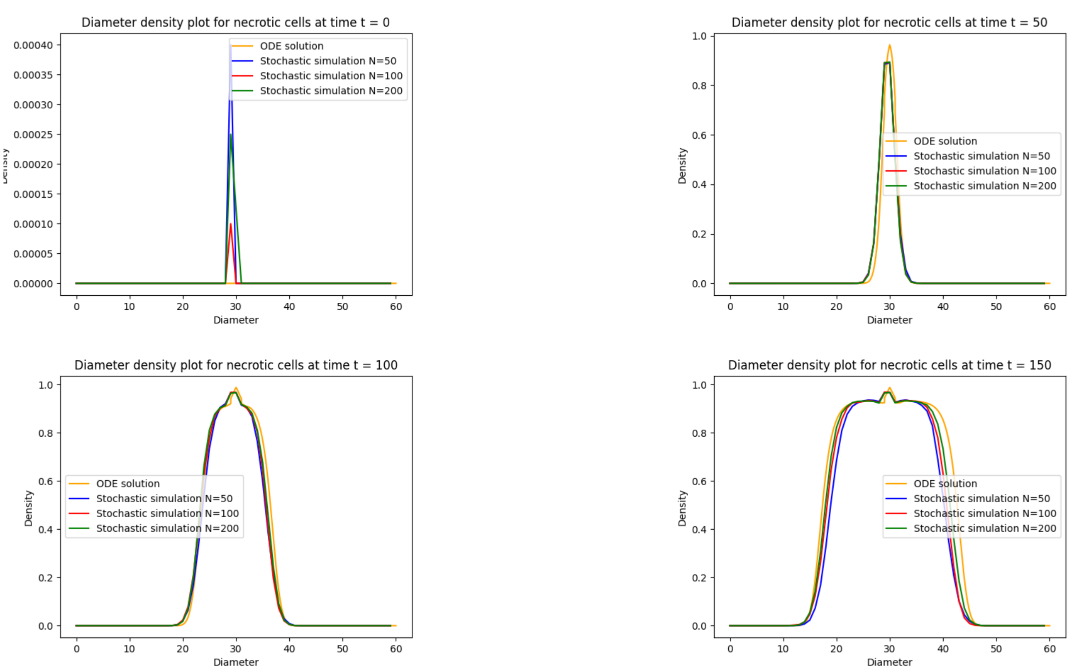
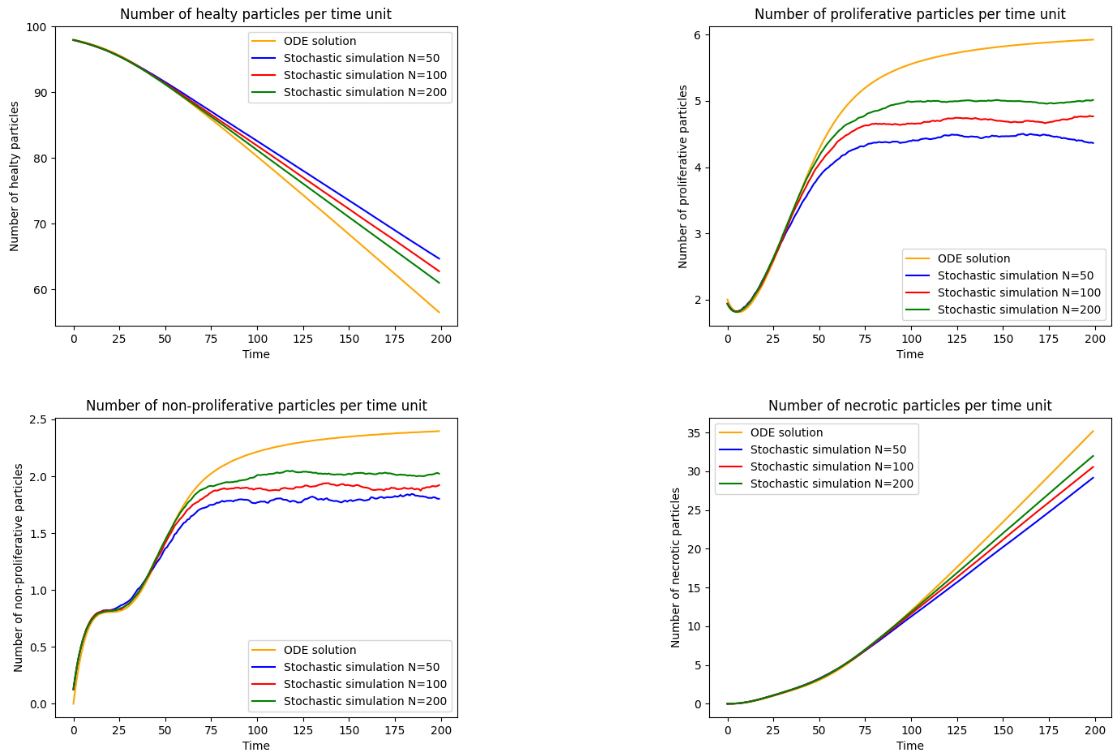


Figure 7.19: Diameter-density plots for necrotic cells of the ODE solution, normal simulation and scaled simulations



Furthermore, we plot the number of the different cells types against the time. We normalize the number of cells in each simulation to compare the results. We find the following number of cells for each of the four types.

Figure 7.20: Number of different type of particles per time unit



In these plots, the convergence becomes clearer. For each particle type the number of particles for the stochastic simulation with $N = 200$ is closest to the number of particles in the ODE solution. The stochastic simulation with $N = 100$ is second best and the simulation for $N = 50$ is the worst. These figures again suggest the convergence of the scaled interacting particle systems to the ODE solution. This is the result we expected.

Chapter 8

Conclusion

In this project, we investigated generally formulated interacting particle systems. These interacting particle systems consist of multiple types of particles and we considered three possible changes that can occur: birth of particles, transition of particles from one type to another and the death of particles. The construction of the generator of this system results in the formulation of the forward Kolmogorov equation describing the stochastic evolution of this system.

The well-posedness of this forward Kolmogorov equation is investigated. By formulating an auxiliary lemma involving a change of variables formula, we were able to determine the exact form of the adjoint operator of the generator of the interacting particle system. This enables us to prove well-posedness in a truncated version of the forward Kolmogorov equation. This result is summarized in Theorem 4.1.4.

Next, we showed both a first moment and second moment estimate as well as a bound on the Boltzmann entropy functional. These a priori estimates and the application of Ascoli-Arzela's Theorem lead to the proof of existence of a solution to the original evolution equation in the weak sense. Furthermore, we established absolute continuity for this solution.

To determine the macroscopic behaviour of generally formulated interacting particle systems, we investigate the mean field limit for this system. To establish the mean field limit we make an additional assumption on rate functions κ_{ij}. The mean field limit is established by scaling the system by N and by taking the limit for N to infinity. The scaling happens by shrinking the grid size by $\frac{1}{N}$. Furthermore, the intensity measure λ is scaled which implies a scaling of mapping $\Lambda^{n,k}$ as well. Computations lead to a system of integro-differential equations. Also for this system well-posedness is established.

Since the interacting particle system is formulated in a general way, the results in this report can be used for many applications. For an interacting particle system with X compact and $\lambda(X) < \infty$ with rate functions satisfying Assumption 2.3.4, the existence of a solution to the forward Kolmogorov equation follows from our results. Furthermore, if the interacting particle is formulated on a $\mathbb{Z}^d$ grid with rate functions additionally satisfying Assumption 6.1.1, this report provides a mean field limit given by a system of integro-differential equations.

We considered an example of an interacting particle system. Tumor growth is described as a multiple type particles system on a compact set in a $\mathbb{Z}^2$ grid. Here, we consider four different types of cells: healthy, proliferative, non-proliferative and necrotic cells. The rates of transitions for each particle depend on the type of the particle itself and the types of particles in a neighbourhood of that particle. The interacting particle system describes the microscopic behaviour of tumor growth.

Using the results for the generally formulated mean field limit, we find the mean field limit for this tumor growth model. Since we specify exact rate functions in this application, we can simulate the solution of this system of integro-differential equations. To compare the interacting particle model and the system of integro-differential equations, we used simulations. We noticed that both the radius-density plots and the number of particles are close for all the models. We also note that the scaled stochastic simulation for $N = 4$ is closest to the ODE solution, whereas the stochastic simulation for

$N = 2$ is the second best fit. This is promising because this is exactly as we would expect. Moreover, we notice a converging trend of the stochastic simulations to the ODE solution.

Nonetheless, we are not completely satisfied with this two-dimensional model. The reason is that we want to investigate the limiting behaviour of the scaled interacting particle system. To numerically determine the ODE solution, discretization of the state space is necessary. This leads to a grid, but since this ODE solution is the limit found by letting the grid size go to zero, we want to consider a grid in the discretization that is much finer than the original interacting particle system. We want a discretization equivalent to a grid after scaling by $N = 1000$. For the two-dimensional model, this results in numerical computations that are too demanding. Therefore, we also investigated a one-dimensional particle system. If we assume spherical symmetry, this one-dimensional particle system can be regarded as the diameter of the tumor. In this one-dimensional system, we were able to discretize, equivalent to scaling with factor $N = 1000$. The convergence is clear in this case, which is promising because it is in line with our expectations.

In future research, the uniqueness of the solution to the forward Kolmogorov equation could be investigated. Existence of the solution is established in Chapter 5 and our conjecture is that this solution is also unique. Moreover, there is a possibility better results for the two-dimensional model can be achieved if the method for solving the ODE is implemented directly, rather than using an ODEsolver in Python.

Nonetheless, the determination of the mean field limit and the convergence in the one-dimensional model are promising results. Due to the general form of the interacting particle system, this result can be used in other applications as well.

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Appendix A

Proof of Lemma 3.1.1

A.1 Proof of Lemma 3.1.1

In this Appendix, we prove Lemma 3.1.1. Before we start proving this statement, we want to introduce a function which helps to shorten our notation.

Definition A.1.1. Let $h(\nu)$ be a $\hat{\Pi}^k(\nu)$-measurable function. We define the function $I_{n_1,\ldots,n_k}(h(\nu))$ as follows

$$I_{n_1,\ldots,n_k}(h(\nu)) := \int_{X^{n_1}} \cdots \int_{X^{n_k}} h(\nu) d\lambda^{\otimes n_1} \ldots d\lambda^{\otimes n_k}.$$

We continue with the proof of Lemma 3.1.1.

Proof of Lemma 3.1.1. In the proof, we are going to split the birth part, the transition part and the death part. We start by proving the birth part holds. We have

$$\int_{\hat{\Gamma}_X} \sum_{m=1}^{k} \int_X F(\nu+\delta_y e_m) g_{0m}(y,\nu)\lambda(dy) d\hat{\Pi}^k(\nu) = \sum_{m=1}^{k} \int_X \int_{\hat{\Gamma}_X} F(\nu+\delta_y e_m) g_{0m}(y,\nu) d\hat{\Pi}^k(\nu)\lambda(dy),$$
$$= \sum_{m=1}^{k} \int_X \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{1}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\ldots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X} \circ \Lambda^{n,k} F(\Lambda^{n,k}+\delta_y e_m) g_{0m}(y,\Lambda^{n,k})\right),$$

In the first step, we apply Fubini's Theorem and then use the definition of the measure $\hat{\Pi}^k(\nu)$. In the following step, we are going to detach the sum over the mth particle from the other sums and prepare to make an index shift. Since the function $g_{0i}(x_{n_m+1},\Lambda^{n_1},\ldots\Lambda^{n_k})$ is zero when $x_{n_m+1} \in \Lambda^{n_i}(\underline{x})$ for some $i \in \{1,\ldots,k\}$ we can include this particle in the indicator function without changing the value of the total expression. Furthermore, in the following expressions we denote

$$n \setminus n_m := n_1,\ldots,n_{m-1},n_{m+1},\ldots,n_k \quad \text{for} \quad m \in \{1,\ldots,k\}.$$

Therefore,

$$= \sum_{m=1}^{k} \sum_{n_m=0}^{\infty} \frac{n_m+1}{(n_m+1)!} \sum_{n\setminus n_m=0}^{\infty} \frac{1}{\prod\limits_{p=1,p\neq m}^{k} n_p!} I_{n_1,\ldots,n_m+1,\ldots,n_k}\Big(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n_1},\ldots,\Lambda^{n_m+1},\ldots,\Lambda^{n_k})$$
$$F(\Lambda^{n_1},\ldots,\Lambda^{n_m+1},\ldots,\Lambda^{n_k}) g_{0m}(x_{n_m+1},\Lambda^{n_1},\ldots,\Lambda^{n_m+1}-\delta_{x_{n_m+1}},\ldots\Lambda^{n_k})\Big),$$

Next, we apply an index shift on the sum over n_m.

$$= \sum_{m=1}^{k} \sum_{n_m=1}^{\infty} \frac{n_m}{(n_m)!} \sum_{n \setminus n_m=0}^{\infty} \frac{1}{\prod\limits_{p=1, p\neq m}^{k} n_p!} I_{n_1,\dots,n_k} \left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) F(\Lambda^{n,k}) g_{0m}(x_{n_m}, \Lambda^{n,k} - \delta_{x_{n_m}} e_m) \right),$$

Since we multiply the entire term within the sum over n_m with n_m we can simply add the case where $n_m = 0$.

$$= \sum_{m=1}^{k} \sum_{n_m=0}^{\infty} \frac{n_m}{(n_m)!} \sum_{n \setminus n_m=0}^{\infty} \frac{1}{\prod\limits_{p=1, p\neq m}^{k} n_p!} I_{n_1,\dots,n_k} \left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) F(\Lambda^{n,k}) g_{0m}(x_{n_m}, \Lambda^{n,k} - \delta_{x_{n_m}} e_m) \right),$$

In the following step, we use a combinatorial trick to get rid of the n_m term. We do this by including a sum from $\ell = 1$ to n_m and considering particle x_ℓ rather than only the last particle x_{n_m}. After this, we use the definition of the measure $\hat{\Pi}^k(\nu)$ again to get to the final result.

$$= \sum_{m=1}^{k} \sum_{n_1,\dots,n_k=0}^{\infty} \frac{1}{\prod\limits_{p=1, p\neq m}^{k} n_p!} I \left(\sum_{\ell=1}^{n_m} \mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) F(\Lambda^{n,k}) g_{0m}(x_\ell, \Lambda^{n_1}, \dots, \Lambda^{n_m} - \delta_{x_\ell}, \dots, \Lambda^{n_k}) \right),$$

$$= \int_{\hat{\Gamma}_X} F(\nu) \sum_{m=1}^{k} \sum_{x \in \nu_m} g_{0m}(x, \nu - \delta_x e_m) d\hat{\Pi}^k(\nu).$$

This proves the birth part of equation (3.1.1) holds. Next, we want to prove the transition part of the lemma holds. First, we interchange sum and integral and apply the definition of the measure $\hat{\Pi}^k(\nu)$.

$$\int_{\hat{\Gamma}_X} \sum_{i,j\neq i}^{k} \sum_{x\in\nu_i} g_{ij}(x,\nu) F(\nu - \delta_x e_i + \delta_x e_j) d\hat{\Pi}^k(\nu)$$

$$= \sum_{i,j\neq i}^{k} \sum_{n_1,\dots,n_k=0}^{\infty} \frac{1}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\dots,n_k} \left(\sum_{\ell=1}^{n_i} \mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) F(\Lambda^{n,k} - \delta_{x_\ell} e_i + \delta_{x_\ell} e_j) g_{ij}(x_\ell, \Lambda^{n,k}) \right),$$

Remark: In the function F, we placed the ith term before the jth term, but this could be interchanged when $j < i$ without loss of generality. In the following step we apply a similar combinatorial trick as in the proof of the birth part but in reversed order. This means that instead of subtracting the Dirac measure of a random particle, we subtract the last particle and multiply with n_i.

$$= \sum_{i,j\neq i}^{k} \sum_{n_1,\dots,n_k=0}^{\infty} \frac{n_i}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\dots,n_k} \left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) F(\Lambda^{n,k} - \delta_{x_{n_i}} e_i + \delta_{x_{n_i}} e_j) g_{ij}(x_{n_i}, \Lambda^{n,k}) \right),$$

Next, we detach the sums over n_i and n_j from the other sums. After this, we apply an index shift over both detached sums.

Furthermore, in the following step we denote $\Lambda^{\tilde{n},k} := (\Lambda^{n_1}, \dots, \Lambda^{n_i - 1}, \dots, \Lambda^{n_j+1}, \dots, \Lambda^{n_k})$ and $n \setminus n_i, n_j := \{n_1, \dots n_k\} \setminus n_i, n_j$.

$$= \sum_{i,j\neq i}^{k} \sum_{n_i=1}^{\infty} \frac{1}{(n_i-1)!} \sum_{n_j=0}^{\infty} \frac{1}{n_j!} \sum_{n\setminus n_i, n_j=0}^{\infty} \frac{1}{\prod\limits_{p=1,p\neq i,j}^{k} n_p!}$$

$$I_{n_1,\ldots,n_i-1,\ldots,n_j+1,\ldots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{\tilde{n},k})F(\Lambda^{\tilde{n},k})g_{ij}(x_{n_j+1},\Lambda^{\tilde{n},k}+\delta_{x_{n_j+1}}e_i-\delta_{x_{n_j+1}}e_j)\right),$$

$$= \sum_{i,j\neq i}^{k} \sum_{n_i=0}^{\infty} \frac{1}{n_i!} \sum_{n_j=1}^{\infty} \frac{1}{(n_j-1)!} \sum_{n\setminus n_i, n_j=0}^{\infty} \frac{1}{\prod\limits_{p=1,p\neq i,j}^{k} n_p!} I_{n_1,\ldots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k})F(\Lambda^{n,k})\right.$$

$$\left. g_{ij}(x_{n_j},\Lambda^{n,k}+\delta_{x_{n_j}}e_i-\delta_{x_{n_j}}e_j)\right),$$

In the following step, we rewrite the expression $\frac{1}{(n_j-1)!}$ to $\frac{n_j}{n_j!}$ and use multiplication with n_j to include the case $n_j = 0$.

$$= \sum_{i,j\neq i}^{k} \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{n_j}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\ldots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k})F(\Lambda^{n,k})g_{ij}(x_{n_j},\Lambda^{n,k}+\delta_{x_{n_j}}e_i-\delta_{x_{n_j}}e_j)\right),$$

We again apply the same combinatorial trick as before and use the definition of measure $\hat{\Pi}^k(\nu)$ in the final step.

$$= \sum_{i,j\neq i}^{k} \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{1}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\ldots,n_k}\left(\sum_{\ell=1}^{n_2} \mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k})F(\Lambda^{n,k})g_{ij}(x_\ell,\Lambda^{n,k}+\delta_{x_\ell}e_i-\delta_{x_\ell}e_j)\right),$$

$$= \int_{\hat{\Gamma}_X} \sum_{i,j\neq i}^{k} \sum_{x\in\nu_j} g_{ij}(x,\nu+\delta_x e_i-\delta_x e_j)d\hat{\Pi}^k(\nu).$$

Thirdly, we want to prove the death part of equation (3.1.1) holds. We again start with using the definition of $\hat{\Pi}^k(\nu)$.

$$\int_{\hat{\Gamma}_X} \sum_{l=1}^{k} \sum_{x\in\nu_l} g_{l0}(x,\nu)F(\nu-\delta_x e_l)d\hat{\Pi}^k(\nu)$$

$$= \sum_{l=1}^{k} \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{1}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\ldots,n_k}\left(\sum_{m=1}^{n_l} \mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k})g_{l0}(x_m,\Lambda^{n,k})F(\Lambda^{n,k}-\delta_{x_m}e_l)\right).$$

The next step is again a result of the similar combinatorial trick used before.

$$= \sum_{l=1}^{k} \sum_{n_1,\ldots,n_k=0}^{\infty} \frac{n_l}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\ldots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k})g_{l0}(x_{n_l},\Lambda^{n,k})F(\Lambda^{n,k}-\delta_{x_{n_l}}e_l)\right).$$

We want to make an index shift again.

$$= \sum_{l=1}^{k} \sum_{n_l=1}^{\infty} \frac{1}{(n_l-1)!} \sum_{n \setminus n_l=0}^{\infty} \frac{1}{\prod\limits_{p=1, p\neq l}^{k} n_p!} I_{n_1,\dots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) g_{l0}(x_{n_l}, \Lambda^{n,k}) F(\Lambda^{n,k} - \delta_{x_{n_l}} e_l \right),$$

$$= \sum_{l=1}^{k} \sum_{n_l=0}^{\infty} \frac{1}{n_l!} \sum_{n \setminus n_l=0}^{\infty} \frac{1}{\prod\limits_{p=1, p\neq l}^{k} n_p!} I_{n_1,\dots,n_l+1,\dots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k} + \delta_{x_{n_l+1}} e_l) g_{l0}(x_{n_l+1}, \Lambda^{n,k} + \delta_{x_{n_l+1}} e_l) F(\Lambda^{n,k}) \right).$$

Lastly, we rewrite this expression and apply the definition of $\hat{\Pi}^k(\nu)$ again.

$$= \sum_{l=1}^{k} \int_X \sum_{n_1,\dots,n_k=0}^{\infty} \frac{1}{\prod\limits_{p=1}^{k} n_p!} I_{n_1,\dots,n_k}\left(\mathbb{1}_{\hat{\Gamma}_X}(\Lambda^{n,k}) g_{l0}(y, \Lambda^{n,k} + \delta_y e_l) F(\Lambda^{n,k}) \right) \lambda(dy)$$

$$= \int_{\hat{\Gamma}_X} \sum_{l=1}^{k} \int_X g_{l0}(y, \nu + \delta_y e_m) \lambda(dy) F(\nu) d\hat{\Pi}^k(\nu).$$

□