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Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint

ISSN 0946 – 8633

**Convergence of stochastic particle systems
undergoing advection and coagulation**

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submitted: December 18, 2012

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No. 1757
Berlin 2012



2010 *Mathematics Subject Classification.* 60K35, 65C35, 82C22.

Key words and phrases. stochastic particle systems, source, outflow, coagulation, advection.

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Abstract

The convergence of stochastic particle systems representing physical advection, inflow, outflow and coagulation is considered. The problem is studied on a bounded spatial domain such that there is a general upper bound on the residence time of a particle. The laws on the appropriate Skorohod path space of the empirical measures of the particle systems are shown to be relatively compact. The paths charged by the limits are characterised as solutions of a weak equation restricted to functions taking the value zero on the outflow boundary. The limit points of the empirical measures are shown to have densities with respect to Lebesgue measure when projected on to physical position space. In the case of a discrete particle type space a strong form of the Smoluchowski coagulation equation with a delocalised coagulation interaction and an inflow boundary condition is derived. As the spatial discretisation is refined in the limit equations, the delocalised coagulation term reduces to the standard local Smoluchowski interaction.

The original Smoluchowski coagulation equation [22] gives a deterministic description of coagulation of an infinite, well-mixed population of particles. Smoluchowski arrived at the equation by considering the volume swept out by a diffusing particle and therefore in some sense from an underlying stochastic model. Heuristic derivations [15, 5], which are more explicitly probabilistic and assume only a general stochastic coagulation process with specified rate, lead via a Kolmogorov forward equation to the same Smoluchowski coagulation equation. An important, and explicit, step in these works is to neglect the correlations between particles. While this assumption was motivated by the need to simplify the problem, it also leads to Markov jump process dynamics that are well suited to simulation [6]. These processes can be used as numerical methods for the Smoluchowski coagulation equation. Rigorous convergence results (existence of a limit point satisfying the Smoluchowski equation) for these stochastic particle methods took some time to develop [9, 16, 2]. Extensive generalisations are now available including general n -particle interactions [3] and [12], the former including particle inflow while the latter provides a CLT result.

Some convergence results are also available that go beyond the assumption of a spatially well mixed population. Guiaş [8] considered coagulation in the presence of diffusion on a spatial lattice and showed convergence of the jump processes to a unique limit point satisfying the Smoluchowski equation ¹ with diffusion. Particles were not able to leave the domains studied. Analogous results for continuous diffusions, that is not on a spatial lattice, were given first by Lang and Xanh [13] and for more general, but still non-degenerate diffusions by Wells [23] and Yaghouti et al. [25].

¹[24] gives a similar result to that in [8], but for a biologically motivated coagulation model that does not lead to the Smoluchowski equation.

Arbitrary Markov free motions and mollified coagulation was included in the rather general work of Kolokoltsov [12], but without boundaries. Reflecting boundary conditions are treated for the closely related mollified Boltzmann equation by Graham and Meleard [7]. However, assumption 2.1 of [7] excludes models where particles can leave the system, because this makes the domain of the generator of the free particle motion too small. Particle exit is also excluded from [14] as a result of the zero gradient boundary condition used. These works did not address the question of how to actually simulate particle transport in a continuous free flow combined with coagulation jumps, nor do they include particle inflow of any kind.

The purpose of the present work is to prove relative compactness (in distribution on the Skorohod space of finite measure valued processes) of a sequence of processes simulating the Smoluchowski coagulation equation with the addition of inception and advective transport in the presence of an outflow boundary. The presence of an active outflow boundary is the key difficulty to be overcome, because this means that there are insufficient functions in the domain of the generator to induce the weak topology. The combination of inception and advection, which are fundamental to the simulation of engineering processes, is also believed to be new. By means of an operator splitting between the advection and coagulation–inception, the Markov processes studied here have been numerically tested in [17], where the results suggest that a limit point exists, as claimed here, and is probably unique. The present work deals only with behaviour as the number of stochastic particles approaches infinity; the spatial discretisation is fixed, corresponding to most of the numerical work [17].

The paper is structured as follows: In §1 there is a description of the particle systems, which suffices to enable a statement of the main results at the end of that section. In §2 the remaining technical details of the processes are presented along with various basic estimates for later use. The section also contains the proof that the processes are defined for all time and are strong Markov; as part of this the ‘piecewise deterministic Markov processes’ of Davis [1] are introduced. Section 3 introduces the empirical measures of the particle systems and a family of Martingales taken from [1] that are used in establishing the relative compactness in distribution of the empirical measures. A weak equation satisfied by the limit measures is derived in §4 and some initial results concerning a density for the limit measures, such a density is a particle concentration, are derived. In particular, for discrete particle type spaces one derives a variant of the Smoluchowski equation with delocalised coagulation. This limit equation reduces to one with the usual local coagulation interaction as the discretisation is refined.

1 Particle Systems and Asymptotic Behaviour

We consider systems of particles in which particles are incepted, coagulate with each other and are carried along by a time-independent flow. A sequence of such particle systems indexed by $n \in \mathbb{N}$ is constructed with the aim of recovering a fluid limit as $n \rightarrow \infty$.

1.1 State Space and Notation

Particles will have positions in a spatial domain $\mathcal{X} = [0, L)$ with closure $\overline{\mathcal{X}} = [0, L]$ and a type, which captures their physical properties and is an element of a locally compact, complete metric space \mathcal{Y} . Addition on \mathcal{Y} is defined to represent the coagulation of two particles. A good example of a type space is $(\mathbb{R}_0^+)^{d_p}$, $d_p \in \mathbb{N}$ where each component represents a different chemical component, but much more complex spaces have also been used in applications [20, 21]. The type encodes all modelled physical properties of a particle such as mass and potentially shape and chemical composition. A further requirement on \mathcal{Y} is the existence of a continuous function $r_1: \mathcal{Y} \rightarrow \mathbb{R}_0^+$ that is sub-additive in the sense that

$$r_1(y_1 + y_2) \leq r_1(y_1) + r_1(y_2) \quad \forall y_1, y_2 \in \mathcal{Y} \quad (1)$$

and for which the sets $\{y \in \mathcal{Y}: r_1(y) \leq A\}$ are compact for every $A \in \mathbb{R}^+$. The function r_1 is thus rather like a norm.

Any number of particles may be present in the system so the state space is the following Fock space:

$$E := \bigcup_{\nu=0}^{\infty} (\mathcal{X} \times \mathcal{Y})^{\nu}, \quad (2)$$

which is locally compact and metrisable. It is given the topology generated by the open sets in the product topology on each of the $(\mathcal{X} \times \mathcal{Y})^{\nu}$, which is locally compact and metrisable (see, for example, [1, §24]) and the associated Borel σ -algebra.

Let $X_n(t) \in E$ be the state of the process with index n at time t and $N(X_n(t))$ the number of particles in its population so that

$$X_n(t) = (X_n(t, i))_{i=1}^{N(X_n(t))} \in E. \quad (3)$$

It is also helpful to write

$$X_n(t, i) = (X_n(t, i, 1), X_n(t, i, 2)) \in \mathcal{X} \times \mathcal{Y} \quad (4)$$

to separate the position and type of a particle. For $X \in E$, a simple point in contrast to the sequence of processes $X_n(t)$, use analogous notation, but without n and t so that $X = ((X(i, 1), X(i, 2)))_{i=1}^{N(X)}$.

We now present some definitions needed to make subsequent statements precise.

Definition 1. Let A be a measurable space, and $A' \subset A$ a measurable subset. $\mathbb{1}_{A'}: A \rightarrow \{0, 1\}$ is the indicator function of A' .

Definition 2. Let A be a subset of \mathbb{R}^d for some $d \in \mathbb{N}$ with the Euclidean topology and associated Borel σ -algebra. Let $C^l(A)$ be the space of continuous functions on A with all derivatives of order upto and including $l \in \mathbb{N}$ bounded and continuous. By convention $C^0(A)$ will be the space of functions that are continuous and bounded.

Definition 3. For the special case $A = \bar{\mathcal{X}} \times \mathcal{Y}$ let

$$C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y}) = \{\psi \in C^0(\bar{\mathcal{X}} \times \mathcal{Y}) : \nabla\psi \in C^0(\bar{\mathcal{X}} \times \mathcal{Y})\}$$

where, as throughout this work, $\nabla\psi(x, y) = \partial_x\psi(x, y)$, because derivatives in the \mathcal{Y} -direction are never considered. This is given the following Sobolev style norm

$$\|\psi\| = \sup_{x,y} |\psi(x, y)| + \sup_{x,y} |\nabla\psi(x, y)|. \quad (5)$$

Definition 4. Let $\mathcal{M}(\bar{\mathcal{X}} \times \mathcal{Y})$ be the space of finite measures on $\bar{\mathcal{X}} \times \mathcal{Y}$.

1.2 Dynamics

1.2.1 Transport

Particles flow through $\mathcal{X} = [0, L)$ at a position (but not type) dependent velocity $u \in C^1(\mathbb{R})$. The velocity u is also required to satisfy

$$u_{-\infty} := \inf_{x \in \mathcal{X}} u(x) > 0, \quad (6)$$

so that the residence time of a particle is bounded. Particles leave the system on reaching L .

1.2.2 Inception

Particles are added to X_n according to a Poisson process on $\bar{\mathcal{X}} \times \mathcal{Y}$ with intensity measure nI where the inception measure I is assumed to satisfy

$$I(\{L\} \times \mathcal{Y}) = 0, \quad (7)$$

$$\int_{\mathcal{X} \times \mathcal{Y}} I(dx, dy) = I(\mathcal{X} \times \mathcal{Y}) = I(\bar{\mathcal{X}} \times \mathcal{Y}) < \infty, \quad (8)$$

$$A_1 := \int_{\mathcal{X} \times \mathcal{Y}} r_1(y) I(dx, dy) < \infty \quad (9)$$

and

$$A_2 := \int_{\mathcal{X} \times \mathcal{Y}} r_1(y)^2 I(dx, dy) < \infty. \quad (10)$$

1.2.3 Coagulation

Coagulation is based on a symmetric, continuous coagulation kernel $K : (\mathcal{X} \times \mathcal{Y})^2 \rightarrow \mathbb{R}_0^+$ with upper bound K_∞ . Two particles $X_n(t, i_1)$ and $X_n(t, i_2)$ coagulate and the enlarged particle is placed in the position of the first particle at rate

$$\sum_{j=1}^J \frac{K(X_n(t, i_1), X_n(t, i_2))}{2\Delta x} \mathbf{1}_{X_j}(X_n(t, i_1, 1)) \mathbf{1}_{X_j}(X_n(t, i_2, 1)). \quad (11)$$

where the $\mathcal{X}_j, j = 1, \dots, J$ form a partition of \mathcal{X} , and for simplicity are taken to be

$$\mathcal{X}_j = [(j-1)\Delta x, j\Delta x) \quad j = 1, \dots, J \quad \Delta x = L/J. \quad (12)$$

This restricts coagulation to particles in the same \mathcal{X}_j , which is convenient during computer simulation. A brief discussion of the placement of the newly coagulated particle may be found in [17].

Recall from §1.1 that coagulation is represented by addition on the type space \mathcal{Y} and that, by (1),

$$\sum_{i=1}^{N(X_n(t))} r_1(X_n(t, i, 2)) \quad (13)$$

does not increase during coagulation events.

1.3 Initial Conditions

Two conditions are placed on the distribution of the initial states $X_n(0)$: Firstly, there must exist $c_0 \geq 0$, such that, for all $0 \leq x_1 \leq x_2 \leq L$,

$$\sum_{i=1}^{N(X_n(0))} \mathbb{1}_{[x_1, x_2]}(X_n(0, i, 1)) \quad (14)$$

is stochastically dominated by $\text{Poi}(nc_0(x_2 - x_1))$. This imposes a basic spatial regularity on the initial condition.

Secondly, for each $l = 0, \dots, d_p$ it is assumed that there exist $A_3, A_4 \geq 0$ such that

$$\mathbb{E} \left[\sum_{i=1}^{N(X_n(0))} r_1(X_n(0, i, 2)) \right] \leq nA_3 \quad (15)$$

and

$$\text{var} \left(\sum_{i=1}^{N(X_n(0))} r_1(X_n(0, i, 2)) \right) \leq nA_4. \quad (16)$$

The purpose of this condition is to ensure tightness of the empirical measures at time 0.

1.4 Main Results

Under the conditions set out in §1.2&1.3 we have the following results, which may be summarised as existence, convergence and characterisation.

Theorem 5. *The $X_n(t)$ are strong Markov processes and, with probability 1, have only a finite number of jumps in any bounded time interval, that is, the processes are defined for all time.*

Theorem 6. *The empirical measure processes $\mu_t^n := \frac{1}{n} \sum_{i=1}^{N(X_n(t))} \delta_{X_n(t,i)}$ of the particle systems form a sequence in the Skorohod space $\mathbb{D}(\mathbb{R}_0^+, \mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y}))$ that is relatively compact in distribution when $\mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y})$ is given the weak topology.*

Theorem 7. *For every $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$ such that $\psi|_{\{L\} \times \mathcal{Y}} \equiv 0$, every limit point μ of the empirical measure processes μ^n satisfies the following weak differential equation with probability 1*

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) \mu_t(dx, dy) = & \\ & \int_{\mathcal{X} \times \mathcal{Y}} u(x) \nabla \psi(x, y) \mu_t(dx, dy) + \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) I(dx, dy) \\ & + \iint_{(\mathcal{X} \times \mathcal{Y})^2} \sum_{j=1}^J [\psi(x_1, y_1 + y_2) - \psi(x_1, y_1) - \psi(x_2, y_2)] \\ & \frac{K(x_1, y_1, x_2, y_2)}{2\Delta x} \mathbb{1}_{\mathcal{X}_j}(x_1) \mathbb{1}_{\mathcal{X}_j}(x_2) \mu_t(dx_1, dy_1) \mu_t(dx_2, dy_2) \end{aligned}$$

and along every convergent sub-sequence μ_0^n converges weakly to μ_0 , also with probability 1. Individual trajectories for finite n deviate from this equation; the mean deviation is $\mathcal{O}(1/n)$ and the fluctuations are $\mathcal{O}(1/\sqrt{n})$.

Theorem 7 specifies an equation solved by almost all trajectories of the limiting process. It does not say that almost all trajectories are identical and the limit is deterministic—this remains an open question, although numerical work [17] has shown no sign of random limits.

Theorem 8. *For every $t \in \mathbb{R}_0^+$ the \mathcal{X} -projection of every limit point μ of the empirical measure processes μ^n is absolutely continuous at t with respect to Lebesgue measure on $\overline{\mathcal{X}}$. In particular, if B is a measurable subset of \mathcal{Y} and $a_1, a_2 \in \overline{\mathcal{X}}$, $a_1 < a_2$, then there exists a function f , parameterised by t and B such that*

$$\mu_t((a_1, a_2) \times B) = \int_{a_1}^{a_2} f(x; t, B) dx.$$

Theorem 8 does not require that the inception measure have a corresponding density, but this is required in order to derive equations for the densities of the limit processes. The availability of a canonical measure on \mathcal{Y} is not assumed so it is in general not meaningful to search for a density of μ_t on $\mathcal{X} \times \mathcal{Y}$. Some partial results involving integrals over \mathcal{Y} are possible, but in the case that \mathcal{Y} is discrete the following result arises:

Theorem 9. *Let \mathcal{Y} be a discrete space endowed with counting measure. Assume that the inception measure I can be decomposed as a sum of two terms, I_{int} , which has a density on $\mathcal{X}^\circ \times \mathcal{Y}$, the interior of the space, and I_{bdry} an inflow boundary component (which would be singular with respect to Lebesgue measure on the whole space) that is supported on $\{0\} \times \mathcal{Y}$. Then with probability 1,*

- 1 for each t , a limit point μ_t has a density c with respect to Lebesgue measure on $\overline{\mathcal{X}}$ and counting measure on \mathcal{Y} ,

2 if c is differentiable in the \mathcal{X} -direction then, for all $x \in \mathcal{X}^\circ$ and $y \in \mathcal{Y}$

$$\begin{aligned} \frac{\partial}{\partial t} c(t, x, y) + \nabla (u(x)c(t, x, y)) &= I_{\text{int}}(x, y) \\ + \frac{1}{2} \sum_{j=1}^J \mathbb{1}_{\mathcal{X}_j}(x) \sum_{\substack{y_1, y_2 \in \mathcal{Y}: \\ y_1 + y_2 = y}} c(t, x, y_1) \int_{\mathcal{X}_j} \frac{dx_2}{\Delta x} K(x, y_1, x_2, y_2) c(t, x_2, y_2) \\ - c(t, x, y) \sum_{j=1}^J \mathbb{1}_{\mathcal{X}_j}(x) \sum_{y_2 \in \mathcal{Y}} \int_{\mathcal{X}_j} \frac{dx_2}{\Delta x} K(x, y, x_2, y_2) c(t, x_2, y_2) \end{aligned}$$

and the following boundary condition holds

$$u(0)c(t, 0, y_1) = I_{\text{bdry}}(y_1).$$

This c , is simply a particle concentration. Under the assumption of \mathcal{X} -differentiability of c one can send $\Delta x \rightarrow 0$ in Theorem 9 and formally recover the Smoluchowski equation with local interaction

$$\begin{aligned} \frac{\partial}{\partial t} c(t, x, y) + \nabla (u(x)c(t, x, y)) &= I_{\text{int}}(x, y) \\ + \frac{1}{2} \sum_{\substack{y_1, y_2 \in \mathcal{Y}: \\ y_1 + y_2 = y}} c(t, x, y_1) K(x, y_1, x_2, y_2) c(t, x_2, y_2) \\ - c(t, x, y) \sum_{y_2 \in \mathcal{Y}} K(x, y, x_2, y_2) c(t, x_2, y_2) \quad (17) \end{aligned}$$

The rate of convergence in Δx for various quantities of theoretical and computational significance of Δx are the subjects of an ongoing study.

2 Details of the Processes

In this section we prove Theorem 5 and establish a number of estimates that are used in the remainder of the analysis.

2.1 Jumps and Associated Notation

Jumps can be divided into two classes: those enforced by the flow (denoted type B in [19]) and spontaneous jumps triggered after Poisson waiting times as is typical for continuous time Markov jump processes (type A in [19]). In this paper, the former category contains only the jumps on particle exit at L ; the latter category comprises inception and coagulation jumps.

2.1.1 Flow and Flow Enforced Exit Jumps

Recall $u \in C^1(\mathbb{R})$. Let $\phi(t; x_0, y_0)$ be the unique solution in $C^1(\mathbb{R}, \mathbb{R} \times \mathcal{Y})$ to

$$\frac{d}{dt}\phi(t; x_0, y_0) = (0, u(\phi(t; x_0, y_0)), 0) \quad \phi(0; x_0, y_0) = (x_0, y_0). \quad (18)$$

This is a flow for a single particle on $\mathbb{R} \times \mathcal{Y} \supset \mathcal{X} \times \mathcal{Y}$. Define $\tilde{\phi}_\nu$ as the flow on $(\mathbb{R} \times \mathcal{Y})^\nu$ that follows ϕ on each copy of $\mathbb{R} \times \mathcal{Y}$.

Definition 10. Let $\tilde{\phi}$ be the flow on $\bigcup_\nu (\mathbb{R} \times \mathcal{Y})^\nu$ such that $\tilde{\phi}|_{(\mathbb{R} \times \mathcal{Y})^\nu} = \tilde{\phi}_\nu$ so that

$$\tilde{\phi}(t; (x_0^i, y_0^i)_{i=1}^\nu) = (\phi(t; x_0^i, y_0^i))_{i=1}^\nu.$$

In between the spontaneous (type A) jumps discussed below the particle systems follows that flow $\tilde{\phi}$ until it meets the boundary of E . This can only occur at time t because a particle reaches L , that is, there exists $i \in \{1, \dots, N(X_n(t))\}$ such that $\lim_{s \rightarrow t} X_n(s, i, 1) = L$, where the limit is taken for $s < t$. Any such particles are removed from the system, in an ‘enforced exit jump’ (a type B jump), which returns the system to the interior of E . The process is then repeated.

Proposition 11. For every $X \in E$ there exists $A_5(X) > 0$ such that $\tilde{\phi}(t, X) \in E$ for all $t < A_5(X)$.

Proof. Let $X = (X(i, 1), X(i, 2))_{i=1}^\nu \in (\mathcal{X} \times \mathcal{Y})^\nu \subset E$ and since $X(i, 1) < L$ for all i then it is sufficient to take

$$A_5(X) = \min \left\{ \frac{L - X(i, 1)}{\sup_{x \in \mathcal{X}} |u(x)|} \mid i = 1, \dots, \nu \right\}. \quad (19)$$

□

The enforced exit jump times will be denoted $S_{n,k} \in \mathbb{R}^+$, $k = 1, \dots, \infty$. The exit counting processes will be denoted $S_n(t) \in \mathbb{N}$. The type of the particle exiting at time $S_{n,k}$ will be denoted $Z_{n,k} \in \mathcal{X} \times \mathcal{Y}$.

2.1.2 Inception

The inception jump times will be denoted $R_{n,k} \in \mathbb{R}^+$, $k = 1, \dots, \infty$. The counting process, which is a Poisson processes with intensity measure nI , will be denoted $R_n(t) \in \mathbb{N}$.

The value in $\mathcal{X} \times \mathcal{Y}$ of the particle incepted at $R_{n,k}$ will be denoted $Y_{n,k}$.

2.1.3 Coagulation

Recall that at rate $K(X_n(t, i_1), X_n(t, i_2)) / (2n\Delta x)$ two particles in cell j coagulate. The detailed transformation is

- $X_n(t, i_2)$ is deleted.
- $N(X_n(t))$ is reduced by 1.
- $X_n(t, i_1)$ is replaced with $(X_n(t, i_1, 1), X_n(t, i_1, 2) + X_n(t, i_2, 2))$.

Particles in different cells do not coagulate with each other by (11).

The following definitions will be used at various places to capture mean and individual effects of coagulations; in these definitions $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$. First, the effect of one coagulation is represented by

$$[\psi]((x_1, y_1), (x_2, y_2)) := [\psi(x_1, y_1 + y_2) - \psi(x_1, y_1) - \psi(x_2, y_2)]. \quad (20)$$

The transition can then be weighted by the coagulation kernel to define

$$[K, \psi]((x_1, y_1), (x_2, y_2)) := \sum_{j=1}^J [\psi]((x_1, y_1), (x_2, y_2)) \frac{K((x_1, y_1), (x_2, y_2))}{\Delta x} \mathbb{1}_{\mathcal{X}_j}(x_1) \mathbb{1}_{\mathcal{X}_j}(x_2). \quad (21)$$

Self coagulations are not considered; the following definition express their effects, which has to be subtracted when (21) is used

$$[[K, \psi]]((x, y)) := [\psi(x, y + y) - 2\psi(x, y)] \frac{K((x, y), (x, y))}{\Delta x}. \quad (22)$$

Average effects are contained in the following operators from functions on $\mathcal{X} \times \mathcal{Y}$ to functions on E (for $X \in E$ the same notation as in §1.1 is used, but without n and t , since only general elements of E , not a sequence of E -valued processes, are under consideration):

$$\mathcal{K}_n \psi(X) = \frac{1}{2n} \sum_{i_1, i_2=1}^{N(X)} [K, \psi](X(i_1), X(i_2)) \quad (23)$$

and self coagulation corrections

$$\tilde{\mathcal{K}}_n \psi(X) = \frac{1}{2n} \sum_{i=1}^{N(X)} [[K, \psi]](X(i)). \quad (24)$$

The coagulation jump times will be denoted $U_{n,k} \in \mathbb{R}^+$, $k = 1, \dots, \infty$. The jump counting process will be $U_n(t) \in \mathbb{N}$. The coagulation event at $U_{n,k}$ will be between the two particles with indices $H_{n,k,1}$ and $H_{n,k,2}$ in that order.

2.1.4 Combined Jump Rate

It is convenient to collect together the rate of all spontaneous jumps as a function λ_n

$$\begin{aligned} \lambda_n(X_n(t)) &= nI(\mathcal{X} \times \mathcal{Y}) \\ &+ \sum_{j=1}^J \sum_{\substack{i_1, i_2=1 \\ i_1 \neq i_2}}^{N(X_n(t))} \frac{K(X_n(t, i_1), X_n(t, i_2))}{2n\Delta x} \mathbb{1}_{\mathcal{X}_j}(X_n(t, i_1, 1)) \mathbb{1}_{\mathcal{X}_j}(X_n(t, i_2, 1)) \end{aligned} \quad (25)$$

and also $\tilde{\lambda}_n \geq \lambda_n$, which includes the rate of the self-coagulations

$$\begin{aligned} \tilde{\lambda}_n(X_n(t)) &= nI(\mathcal{X} \times \mathcal{Y}) \\ &+ \sum_{j=1}^J \sum_{i_1, i_2=1}^{N(X_n(t))} \frac{K(X_n(t, i_1), X_n(t, i_2))}{2n\Delta x} \mathbb{1}_{\mathcal{X}_j}(X_n(t, i_1, 1)) \mathbb{1}_{\mathcal{X}_j}(X_n(t, i_2, 1)) \end{aligned} \quad (26)$$

Proposition 12. *The λ_n and $\tilde{\lambda}_n$ are measurable and, for every $X \in E$*

$$\int_0^{A_5(X)} \tilde{\lambda}_n(\tilde{\phi}(t; X)) dt < \infty.$$

Proof. Measurability is immediate from the construction using simpler measurable functions. If X contains N particles, then $\tilde{\phi}(t; X)$ will also have N particles during $[0, A_5(X))$ and hence on the same time interval

$$\tilde{\lambda}_n(\tilde{\phi}(t; X)) \leq nI(\mathcal{X} \times \mathcal{Y}) + \frac{K_\infty}{2n\Delta x} N^2. \quad (27)$$

□

Definition 13. $T_n(t) := R_n(t) + S_n(t) + U_n(t)$ is the jump counting process.

2.2 Piecewise Deterministic Markov Processes

A few simple estimates are now presented. They will be useful at various point in the analysis which follows. In particular they imply the “standard conditions” of Davis [1, (24.8)] are fulfilled so that the X_n are càdlàg strong Markov processes (although in general not Feller) and have no explosion of jumps thus proving Theorem 5.

Proposition 14. *There can be no explosion of jumps in the processes defined above. In fact, for all $t \geq 0$ and $l \in \mathbb{N}$, there exist $A_6(t, l), A_7(t, l) \in \mathbb{R}^+$ such that*

$$\mathbb{E} \left[\left(\frac{T_n(t)}{n} \right)^l \middle| X_n(0) \right] \leq A_6(t, l) + 2^{l-1} N(X_n(0))$$

and

$$\mathbb{E} \left[\left(\frac{T_n(t)}{n} \right)^l \right] \leq A_7(t, l).$$

Proof. Since particles can exit at most once and every coagulation removes one particle

$$\begin{aligned} T_n(t) &= R_n(t) + S_n(t) + U_n(t) \\ &\leq R_n(t) + (R_n(t) + N(X_n(0))) \\ &\leq 2R_n(t) + N(X_n(0)). \end{aligned}$$

Now $R_n(t)$ is Poisson with mean $ntI(\mathcal{X} \times \mathcal{Y})$ and $N(X_n(0))$ is stochastically dominated by a Poisson random variable with mean nc_0L , see (14). □

Proposition 15. *The total number of particles has polynomial moments: For all $t \geq 0$ and $l \in \mathbb{N}$ there exists $A_8(t, l) \in \mathbb{R}^+$ such that for all $n \in \mathbb{N}$*

$$\mathbb{E} \left[\left(\frac{\sup_{s \leq t} N(X_n(s))}{n} \right)^l \right] \leq A_8(t, l).$$

Proof. The only process that increases the number of particles is inception hence

$$\sup_{s \leq t} N(X_n(s)) \leq N(X_n(0)) + R_n(t).$$

Since $R_n(t)$ is non-decreasing in time, observing the Poisson distribution of $R_n(t)$ and the stochastic domination of $N(X_n(0))$ completes the proof, since the result holds for Poisson distributed random variables. \square

Proposition 16. *For all $t \geq 0$ and $\epsilon > 0$, there exists $A_9(t, \epsilon) \in \mathbb{R}^+$ such that*

$$\mathbb{P} \left(\sup_{s \leq t} \frac{N(X_n(s))}{n} \geq A_9(t, \epsilon) \right) \leq \frac{\epsilon}{n}.$$

Further, if the X_n are defined on a common probability space, there also exists $A_{10}(t) \in \mathbb{R}^+$ such that

$$\mathbb{P} \left(\sup_{s \leq t} \frac{N(X_n(s))}{n} \leq A_{10}(t) \text{ ult.} \right) = 1,$$

where

$$\left\{ \sup_{s \leq t} \frac{N(X_n(s))}{n} \leq A_{10}(t) \text{ ult.} \right\} = \bigcup_{n_0} \bigcap_{n \geq n_0} \left\{ \sup_{s \leq t} \frac{N(X_n(s))}{n} \leq A_{10}(t) \right\}$$

is the event that the bound is satisfied for all n large enough, where the definition of large enough may itself be random, but finite.

Proof. Let $t \geq s \geq 0$ then

$$N(X_n(s)) \leq N(X_n(0)) + R_n(s) \leq N(X_n(0)) + R_n(t),$$

since $R_n(t)$ has non-decreasing paths to see that $\sup_{s \leq t} N(X_n(s))$ is stochastically dominated by a Poisson random variable with mean $nc_0L + ntI(\mathcal{X} \times \mathcal{Y})$. Now take

$$A_9(t, \epsilon) = c_0L + tI(\mathcal{X} \times \mathcal{Y}) + \sqrt{\frac{c_0L + tI(\mathcal{X} \times \mathcal{Y})}{\epsilon}}$$

and apply Proposition 42 to derive the first statement of the proposition.

For the second statement take

$$A_{10}(t) = e(c_0L + tI(\mathcal{X} \times \mathcal{Y})) \tag{28}$$

and use Proposition 43 and Borel-Cantelli. No assumption about independence (or dependence) between the X_n is required for the application of Borel-Cantelli. In particular, if the processes are not defined on a common probability space, a product space may be used. \square

Proposition 17. *The jump rate has polynomial moments: For all $t \geq 0$ and $l \in \mathbb{N}$ there exists $A_{11}(t, l)$ such that for all $n \in \mathbb{N}$*

$$\mathbb{E} \left[\left(\frac{\sup_{s \leq t} \tilde{\lambda}_n(X_n(s))}{n} \right)^l \right] \leq A_{11}(t, l).$$

Proof. Note that for $s \geq 0$

$$\frac{\tilde{\lambda}_n(X_n(s))}{n} \leq I(\mathcal{X} \times \mathcal{Y}) + \frac{K_\infty}{2n^2 \Delta x} N(X_n(s))^2$$

and hence

$$\begin{aligned} \mathbb{E} \left[\left(\frac{\sup_{s \leq t} \tilde{\lambda}_n(X_n(s))}{n} \right)^l \right] \\ \leq 2^{l-1} I(\mathcal{X} \times \mathcal{Y})^l + 2^{l-1} \left(\frac{K_\infty}{2\Delta x} \right)^l \mathbb{E} \left[\left(\frac{\sup_{s \leq t} N(X_n(s))}{n} \right)^{2l} \right] \end{aligned}$$

and the result follows from Proposition 15. Note that this result is stated and proved for $\tilde{\lambda}_n$ which is an upper bound for λ_n . \square

Proof of Theorem 5. This proof consists of showing that the four ‘standard conditions’ of [1, §24.8] are satisfied and so [1, Theorem 25.5], which asserts the strong Markov property, applies. The fourth condition is non-explosion, which is Proposition 14, which also covers the additional part of the Theorem 5 of the present work. The second condition is Proposition 12. The third condition is checked in Proposition 41, which is placed in Appendix A along with definitions of the notation that seems to be necessary for this purpose only. The remaining condition requires the the operator generating the flows $\tilde{\phi}$ is locally Lipschitz on C^∞ , which is immediate. \square

3 Empirical Measures

Before considering the empirical measures themselves, we consider a family of Martingales which are key to proving the necessary results concerning the empirical measures.

3.1 Martingales

The generator of a general piecewise deterministic Markov process is given in [1, 26.14]. However, the domain of such generators places boundary conditions on the functions to which the generator can be applied because of the flow enforced jumps. Something slightly more general than Dynkin’s formula is then required to construct the martingales that are a key technical tool

in this paper. The necessary generalisation is simply the subtraction of the effects of the flow enforced jumps. The martingales, which are based on sums over all particles, will now be built up in stages.

Let $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$ the space of continuous bounded real-valued functions on $\overline{\mathcal{X}} \times \mathcal{Y}$, which also have a continuous bounded derivative in the \mathcal{X} direction. Let $\psi^\oplus : E \rightarrow \mathbb{R}$ be defined by

$$\psi^\oplus|_{(\mathcal{X} \times \mathcal{Y})^\nu}(z) = \sum_{i=1}^{\nu} \psi(x(i), y(i)), \quad z = (x(i), y(i))_{i=1}^{\nu} \in (\mathcal{X} \times \mathcal{Y})^\nu \subset E \quad (29)$$

This notation is taken from [12].

Define

$$\begin{aligned} M_n^\psi(t) &:= \frac{1}{n} \psi^\oplus(X_n(t)) - \frac{1}{n} \psi^\oplus(X_n(0)) \\ &+ \frac{1}{n} \sum_{k=1}^{S_n(t)} \psi(L, Z_{n,k}) - \frac{1}{n} \int_0^t \mathcal{K}_n \psi(X_n(s)) ds + \frac{1}{n} \int_0^t \tilde{\mathcal{K}}_n \psi(X_n(s)) ds \\ &\quad - t \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) I(dx, dy) - \frac{1}{n} \int_0^t (u \nabla \psi)^\oplus(X_n(s)) ds, \end{aligned} \quad (30)$$

where, as throughout this work, ∇ acts only in the \mathcal{X} direction, and

$$\begin{aligned} \widehat{M}_n^\psi(t) &:= \frac{1}{n} \sum_{k=1}^{R_n(t)} \psi(Y_{n,k}) - t \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) I(dx, dy) \\ &\quad + \frac{1}{n} \sum_{k=1}^{U_n(t)} [\psi](X_n(U_{n,k}-, j, H_{n,k,1}), X_n(U_{n,k}-, j, H_{n,k,2})) \\ &\quad - \frac{1}{n} \int_0^t \mathcal{K}_n \psi(X_n(s)) ds + \frac{1}{n} \int_0^t \tilde{\mathcal{K}}_n \psi(X_n(s)) ds, \end{aligned} \quad (31)$$

where $U_{n,k}-$ indicates the limit from the left, that is, the state immediately before the coagulation jump at $U_{n,k}$.

By Davis [1, Theorems 26.12 & 31.3] M_n^ψ and \widehat{M}_n^ψ are almost surely equal to each other and martingales in the filtration generated by the underlying process.

The next results will show that these martingales converge to 0 as $n \rightarrow \infty$. As a first step local square integrability is established.

Proposition 18. *For all $t \geq 0$ and $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$ there exists $A_{12}(t, \psi) \in \mathbb{R}^+$ independent of n such that*

$$\mathbb{E} \left[\widehat{M}_n^\psi(t)^2 \right] \leq A_{12}(t, \psi).$$

Proof. Since $(a + b)^2 \leq 2(a^2 + b^2)$

$$\begin{aligned}
\widehat{M}_n^\psi(t)^2 &\leq 2 \left(\frac{1}{n} \sum_{k=1}^{R_n(t)} \psi(Y_{n,k}) + \right. \\
&\quad \left. \frac{1}{n} \sum_{k=1}^{U_n(t)} [\psi](X_n(U_{n,k}^-, H_{n,k,1}), X_n(U_{n,k}^-, H_{n,k,2})) \right)^2 \\
&+ 2 \left(t \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) I(dx, dy) + \right. \\
&\quad \left. \frac{1}{n} \int_0^t \mathcal{K}_n \psi(X_n(s)) ds - \frac{1}{n} \int_0^t \tilde{\mathcal{K}}_n \psi(X_n(s)) ds \right)^2 \\
&\leq 2 \left(\frac{3 \|\psi\|}{n} T_n(t) \right)^2 + 2 \left(\frac{3 \|\psi\|}{n} \int_0^t \tilde{\lambda}_n(X_n(s)) ds \right)^2 \\
&\leq \frac{18 \|\psi\|^2}{n^2} \left(T_n(t)^2 + t^2 \sup_{s \leq t} \tilde{\lambda}_n(X_n(s))^2 \right)
\end{aligned}$$

and one can now apply Proposition 14 and Proposition 17. \square

Proposition 19. For all $t \geq 0$ and $\psi \in C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y})$ there exists $A_{13}(t, \psi)$, independent of n such that

$$\mathbb{E} \left[\widehat{M}_n^\psi(t)^2 \right] \leq \frac{A_{13}(t, \psi)}{n}.$$

Proof. Proposition 18 establishes the applicability of Proposition 44, which shows

$$\begin{aligned}
&\mathbb{E} \left[\left(\widehat{M}_n^\psi(t) - \widehat{M}_n^\psi(0) \right)^2 \right] \\
&= \sum_{k=1}^{\infty} \mathbb{E} \left[\left(\widehat{M}_n^\psi(t \wedge T_{n,k}) - \widehat{M}_n^\psi(t \wedge T_{n,k-1}) \right)^2 \right] \\
&= \mathbb{E} \left[\sum_{k=1}^{T_n(t)} \left(\widehat{M}_n^\psi(T_{n,k}) - \widehat{M}_n^\psi(T_{n,k-1}) \right)^2 \right] + \mathbb{E} \left[\left(\widehat{M}_n^\psi(t) - \widehat{M}_n^\psi(T_{n,T_n(t)}) \right)^2 \right]. \quad (32)
\end{aligned}$$

But, because there is one jump in $[T_{n,k-1}, T_{n,k}]$ (which must be at $T_{n,k}$) one has

$$\left| \widehat{M}_n^\psi(T_{n,k}) - \widehat{M}_n^\psi(T_{n,k-1}) \right| \leq \frac{3 \|\psi\|}{n} \left(1 + \int_{T_{n,k-1}}^{T_{n,k}} \lambda_n(X_n(s)) ds \right). \quad (33)$$

Hence

$$\begin{aligned}
&\mathbb{E} \left[\left(\widehat{M}_n^\psi(T_{n,k}) - \widehat{M}_n^\psi(T_{n,k-1}) \right)^2 \right] \\
&\leq \frac{18 \|\psi\|^2}{n^2} \mathbb{E} \left[1 + \left(\int_{T_{n,k-1}}^{T_{n,k}} \lambda_n(X_n(s)) ds \right)^2 \right] \quad (34)
\end{aligned}$$

and

$$\begin{aligned} \mathbb{E} \left[\left(\widehat{M}_n^\psi(t) - \widehat{M}_n^\psi(T_{n,T_n(t)}) \right)^2 \right] \\ \leq \frac{18 \|\psi\|^2}{n^2} \mathbb{E} \left[\left(\int_{T_n, T_n(t)}^t \lambda_n(X_n(s)) ds \right)^2 \right]. \end{aligned} \quad (35)$$

However, $\lambda_n(X_n(s))$ is the rate at which coagulation and inception jumps occur. Hence $T_{n,k} - T_{n,k-1}$ is the minimum of a waiting time with (deterministic conditional on $X_n(T_{n,k-1})$ rate $\lambda_n(X_n(s))$ and the next flow enforced jump, so

$$\int_{T_{n,k-1}}^{T_{n,k}} \lambda_n(X_n(s)) ds \quad (36)$$

is stochastically dominated by an exponential random variable with mean 1 and second moment 2. Thus

$$\begin{aligned} \mathbb{E} \left[\left(\widehat{M}_n^\psi(t) - \widehat{M}_n^\psi(0) \right)^2 \right] &\leq \frac{18 \|\psi\|^2}{n^2} \mathbb{E} \left[\sum_{l=1}^{T_n(t)+1} 3 \right] \\ &= \frac{54 \|\psi\|^2}{n^2} \mathbb{E} [T_n(t) + 1] \end{aligned} \quad (37)$$

and the result follows since Proposition 14 shows that $\mathbb{E} [T_n(t)] / n$ has a bound that is independent of n . \square

An immediate consequence of this result is that:

Proposition 20. For all $t \geq 0$ and $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$

$$\mathbb{E} \left[\sup_{s \leq t} \widehat{M}_n^\psi(s)^2 \right] \leq \frac{4A_{13}(t, \psi)}{n}.$$

Proof. Doob's inequality (see, for example, [4, Chapter 2, Proposition 2.16b]) or [11, Proposition 7.16]). \square

3.2 Coordinate Projections

The explicit construction of the X_n and then of \widehat{M}_n provides a way to prove many of the estimates in the following sections. The focus now moves from the X_n to the associated empirical measures. This factors out the different orderings of particles and the problem that a limit $\lim_{n \rightarrow \infty} X_n$ might not be an E -valued process, because it could have an infinite number of particles.

Definition 21. The empirical measure process of the particle system X_n is defined as a sum of Dirac-masses by

$$\mu_t^n := \frac{1}{n} \sum_{i=1}^{N(X_n(t))} \delta_{X_n(t,i)}.$$

For any measurable space A , measure μ on A and measurable function $\psi: A \rightarrow \mathbb{R}$ let

$$\langle \psi, \mu \rangle := \int_A \psi(a) d\mu(a). \quad (38)$$

The pairings $\langle \psi, \mu_t^n \rangle$ are called the co-ordinate projections of the empirical measures and are elements of $\mathbb{D}(\mathbb{R}_0^+, \mathbb{R})$. The properties of these projections are now studied for $\psi \in C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y})$.

The martingales (30) may be rearranged to show

$$\begin{aligned} \langle \psi, \mu_t^n \rangle &= \langle \psi, \mu_0^n \rangle + \int_0^t \langle u \nabla \psi, \mu_s^n \rangle ds + t \langle \psi, I \rangle \\ &\quad + \frac{1}{2} \int_0^t \langle [K, \psi], \mu_s^n \otimes \mu_s^n \rangle ds - \frac{1}{2n} \int_0^t \langle [[K, \psi]], \mu_s^n \rangle ds \\ &\quad - \frac{1}{n} \sum_{k=1}^{S_n(t)} \psi(L, Z_{n,k}) + M_n^\psi(t). \end{aligned} \quad (39)$$

Definition 22. Since $\inf_x u(x) > 0$, exit times

$$\mathcal{T}_x := \inf \{ t \geq 0 : \phi(t; x, y) \in (\bar{\mathcal{X}} \setminus \mathcal{X}) \times \mathcal{Y} \}, \quad x \in \mathcal{X}, \quad (40)$$

which do not depend on y due to (18), are differentiable with $\frac{d}{dx} \mathcal{T}_x = -u(x) < 0$ and $\sup_{x \in \mathcal{X}} \mathcal{T}_x = \mathcal{T}_0 < \infty$.

As a preliminary step to proving the required bound on the modified variation of the coordinate projections, the variation on one fixed time interval is considered:

Proposition 23. For all $t \geq 0, \epsilon > 0, \eta > 0$ and $\psi \in C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y})$, there exists $A_{14}(t, \psi, \eta, \epsilon) \in \mathbb{R}^+$ such that, if $0 \leq t_1 < t_2 \leq t$ and $t_2 - t_1 \leq A_{14}(t, \psi, \eta, \epsilon)$

$$\mathbb{P}(|\langle \psi, \mu_{t_2}^n \rangle - \langle \psi, \mu_{t_1}^n \rangle| \geq \eta) \leq \frac{\epsilon}{n}.$$

Proof. Use (39) to show that

$$\begin{aligned} &|\langle \psi, \mu_{t_2}^n \rangle - \langle \psi, \mu_{t_1}^n \rangle| \\ &\leq (t_2 - t_1) \left[\|\psi\| I(\mathcal{X} \times \mathcal{Y}) + \left(\|u \nabla \psi\| + \frac{3K_\infty \|\psi\|}{2n} \right) \sup_{s \leq t} \mu_s^n(\mathcal{X} \times \mathcal{Y}) \right. \\ &\quad \left. + \frac{3K_\infty \|\psi\|}{2} \sup_{s \leq t} \mu_s^n(\mathcal{X} \times \mathcal{Y})^2 \right] \\ &\quad + \|\psi\| \frac{S_n(t_2) - S_n(t_1)}{n}. \end{aligned}$$

By Proposition 16 the probability that the term including the square brackets exceeds $\frac{\eta}{2}$ is at most $\frac{\epsilon}{2n}$ provided

$$(t_2 - t_1) \leq \frac{\frac{\eta}{2}}{\|\psi\| I(\mathcal{X} \times \mathcal{Y}) + \left(\|u \nabla \psi\| + \frac{3K_\infty \|\psi\|}{2n} \right) A_9(t, \epsilon/2) + \frac{3K_\infty \|\psi\|}{2} A_9(t, \epsilon/2)^2}.$$

$S_n(t_2) - S_n(t_1)$ is the number of particles leaving the system during the time interval $(t_1, t_2]$. These can be broken down into the contributions of particles that entered the system as a result of inception events at some positive time, $\Delta S'$, the contributions of particles present at time 0, $\Delta S''$. For a particle incepted at time τ at position x and exiting the system in the $(t_1, t_2]$ one must have

$$t_1 < \tau + \mathcal{T}_x \leq t_2. \quad (41)$$

Not all particles satisfying this condition will exit the system in the indicated time interval—some will be consumed in coagulation events, but this shows that $S_n(t_2) - S_n(t_1)$ is stochastically dominated by a Poisson random variable with mean

$$n \int_0^t \int_{\mathcal{X} \times \mathcal{Y}} \mathbb{1}(t_1 < \tau + \mathcal{T}_x \leq t_2) I(dx, dy) d\tau \leq n(t_2 - t_1) I(\mathcal{X} \times \mathcal{Y}). \quad (42)$$

Hence, by Proposition 42

$$\mathbb{P} \left(\frac{\Delta S'}{n} \geq \frac{\eta}{4 \|\psi\|} \right) \leq \frac{\epsilon}{4n}, \quad (43)$$

provided

$$t_2 - t_1 \leq \frac{1}{2I(\mathcal{X} \times \mathcal{Y})} \left(\frac{\eta}{2 \|\psi\|} + \frac{1}{\epsilon} \left(1 - \sqrt{1 + \frac{\epsilon \eta}{\|\psi\|}} \right) \right). \quad (44)$$

Finally, particles that were present at time 0 may also leave the system. The mapping from particle position to remaining residence time, $x \mapsto \mathcal{T}_x$ (see §2.1.1) has a strictly negative derivative and a differentiable inverse when regarded as a map $[0, L] \rightarrow [0, \mathcal{T}_0]$. The derivative of this inverse is bounded away from 0 by $-1/\inf_{x \in \mathcal{X}} u(x)$ and hence $\Delta S''$ is stochastically bounded by $\text{Poi}(n(t_2 - t_1)c_0/\inf_{x \in \mathcal{X}} u(x))$, which further yields

$$\mathbb{P} \left(\frac{\Delta S''}{n} > \frac{\eta}{4 \|\psi\|} \right) \leq \frac{\epsilon}{4n}, \quad (45)$$

provided

$$t_2 - t_1 \leq \frac{\inf_{x \in \mathcal{X}} u(x)}{2c_0} \left(\frac{\eta}{2 \|\psi\|} + \frac{1}{\epsilon} \left(1 - \sqrt{1 + \frac{\epsilon \eta}{\|\psi\|}} \right) \right). \quad (46)$$

□

A majorant variation, which dominates the modified variation is now defined explicitly to provide a direct way to achieve an upper bound for the modified variation.

Definition 24. Let f be a function from \mathbb{R}^+ into a metric space with metric ρ . For h such that $t > h > 0$, define $P = P(h) = \lfloor t/h \rfloor$, $t_p = ph$, $p = 0, \dots, P-1$ and $t_P = t$ so that $t_{p+1} - t_p < 2h \forall p \in \{1, \dots, P-1\}$.

Using this partition define the majorant variation of f by

$$\tilde{v}(f, t, h) := \max_p \sup_{r, s \in [t_p, t_{p+1})} \rho(f(r), f(s)). \quad (47)$$

Proposition 25. For every $T > 0$, $\eta > 0$ and $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$, there exists $h > 0$ such that, regarding $\langle \psi, \mu^n \rangle$ as a function of t so that $\langle \psi, \mu^n \rangle(t) = \langle \psi, \mu_t^n \rangle$

$$\mathbb{P}(\tilde{v}(\langle \psi, \mu^n \rangle, T, h) \geq \eta) \leq \frac{\eta}{n}. \quad (48)$$

Proof. Let $0 < h < A_{14}(T, f, \eta, \epsilon/P(h))/2$ so that no element in the partition from Definition 24 has length more than $A_{14}(T, f, \eta, \eta/P(h))$, then

$$\begin{aligned} & \mathbb{P}(\tilde{v}(\langle \psi, \mu^n \rangle, T, h) \geq \eta) \\ & \leq \sum_{p=1}^{P(h)} \mathbb{P}\left(\sup_{\substack{s_1, s_2 \in [t_{p-1}, t_p) \\ s_1 < s_2}} |\langle \psi, \mu_{s_2}^n \rangle - \langle \psi, \mu_{s_1}^n \rangle| \geq \eta\right) \leq P(h) \frac{\eta}{nP(h)} = \frac{\eta}{n}. \end{aligned} \quad (49)$$

□

Proposition 26. For each $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$ the processes $\langle \psi, \mu_t^n \rangle$ form a sequence in $\mathbb{D}(\mathbb{R}^+, \mathbb{R})$ that is relatively compact in distribution.

Proof. Proposition 16 and Proposition 25 satisfy the conditions for relative compactness with càdlàg limits from [4, Chapter 3, Corollary 7.4]. □

3.3 Compact Containment

Recall that $\mathcal{A} \subset \mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y})$ is tight (in the weak topology) if

- $\sup_{\mu \in \mathcal{A}} \mu(\overline{\mathcal{X}} \times \mathcal{Y}) < \infty$, and
- for all $\eta > 0$ one can find a compact set $B_\eta \subset \overline{\mathcal{X}} \times \mathcal{Y}$ such that $\sup_{\mu \in \mathcal{A}} \mu(B_\eta^c) < \eta$.

Appropriate compact set B_η will now be constructed by considering the the inception process. Recall the following notation: for $(x, y) \in \mathcal{X} \times \mathcal{Y}$, y_l is the l -th component of y and $y_0 \equiv 1$ so that component '0' provides a way of counting the number of particles.

Definition 27. The total amount of r_1 incepted upto time t is

$$\widehat{W}_n(t) := \sum_{k=0}^{R_n(t)} r_1(Y_{n,k,2}).$$

Proposition 28.

$$\mathbb{E} \left[\widehat{W}_n(t) \right] = ntA_1$$

and

$$\text{var} \left(\widehat{W}_n(t) \right) = ntA_2.$$

Proof. Refer to (9)&(10) where the constants are defined and condition on the number of inception events. \square

Proposition 29. For all $t \geq 0, \epsilon > 0$ there exists $A_{15}(t, \epsilon) \in \mathbb{R}^+$ such that, for all $n \in \mathbb{N}$

$$\mathbb{P} \left(\sup_{s \leq t} \langle r_1, \mu_s^n \rangle > A_{15}(t, \epsilon) \right) \leq \frac{\epsilon}{n}$$

Proof. Note that, with probability 1,

$$n \sup_{s \leq t} \langle r_1, \mu_s^n \rangle \leq \sum_{i=1}^{N_n(X_n(0))} r_1(X_n(0, i, 2)) + \widehat{W}_n(t). \quad (50)$$

The right hand side of (50) has mean at most $nA_3 + ntA_1$ and variance at most $nA_4 + ntA_2$. So let

$$A_{15}(t, \epsilon) = A_3 + tA_1 + \sqrt{\frac{A_4 + tA_2}{\epsilon}} \quad (51)$$

and apply Proposition 42. \square

Compact sets are now constructed in $\overline{\mathcal{X}} \times \mathcal{Y}$ and the measure space $\mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y})$

Definition 30. The following set is compact by assumption (see §1.1):

$$B_{t, \epsilon, \eta} := \left\{ (x, y) \in \overline{\mathcal{X}} \times \mathcal{Y} : r_1(y) \leq \frac{2A_{15}(t, \epsilon/2)}{\eta} \right\}.$$

Definition 31. For the space of measures, let

$$C_{t, \epsilon} := \bigcap_{q \in \mathbb{Q}^+} \left\{ \mu \in \mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y}) : \mu(\overline{\mathcal{X}} \times \mathcal{Y}) \leq A_9(t, \epsilon/2), \mu(B_{t, \epsilon, q}^c) < q \right\}.$$

By construction, $C_{t, \epsilon}$ is tight and therefore has a compact closure in $\mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y})$. The task is therefore to show that the probability of μ_s^n leaving $C_{t, \epsilon}$ before time t is at most η . It is helpful to note that, because all particles have positions in \mathcal{X} , $\mu_t^n(\mathcal{X} \times \mathcal{Y}) = \mu_t^n(\overline{\mathcal{X}} \times \mathcal{Y})$ for all t and n .

Proposition 32. For all $t \geq 0$ and $\epsilon > 0$

$$\mathbb{P}(\mu_s^n \in C_{t, \epsilon} \forall s \leq t) \geq 1 - \frac{\epsilon}{n}.$$

Proof. First note that for any $q \in \mathbb{Q}^+$ and $t \geq 0$

$$\sup_{s \leq t} \langle r_1, \mu_s^n \rangle \geq \frac{2A_{15}(t, \epsilon/2)}{q} \sup_{s \leq t} \mu_s^n (B_{t, \epsilon, q}^c) \quad (52)$$

and thus

$$\begin{aligned} \left\{ \sup_{s \leq t} \langle r_1, \mu_s^n \rangle \leq A_{15}(t, \epsilon/2) \right\} &\subset \left\{ \sup_{s \leq t} \langle r_1, \mu_s^n \rangle < 2A_{15}(t, \epsilon/2) \right\} \\ &\subset \left\{ \sup_{s \leq t} \mu_s^n (B_{t, \epsilon, q}^c) < q \right\} \subset \bigcap_{q' \in \mathbb{Q}^+} \left\{ \sup_{s \leq t} \mu_s^n (B_{t, \epsilon, q'}^c) < q' \right\} \end{aligned} \quad (53)$$

so that, by Proposition 29

$$1 - \frac{\epsilon}{n} \leq \mathbb{P} \left(\sup_{s \leq t} \langle r_1, \mu_s^n \rangle \leq A_{15}(t, \epsilon) \right) \leq \mathbb{P} \left(\bigcap_{q' \in \mathbb{Q}^+} \{ \mu_s^n (B_{t, \epsilon, q'}^c) < q' \} \right). \quad (54)$$

Then

$$\begin{aligned} &\mathbb{P} (\mu_s^n \in C_{t, \eta} \forall s \leq t) \\ &\geq \mathbb{P} \left(\bigcap_{q \in \mathbb{Q}} \left\{ \sup_{s \leq t} \mu_s^n (B_{t, \eta, q}^c) < q \right\} \cap \left\{ \sup_{s \leq t} \mu_s^n (\mathcal{X} \times \mathcal{Y}) \leq A_9(t, \eta) \right\} \right) \end{aligned} \quad (55)$$

and using (54) and Proposition 16

$$1 - \mathbb{P} (\mu_s^n \in C_{t, \eta} \forall s \leq t) \leq \frac{\epsilon}{n} \quad (56)$$

□

3.4 Relative Compactness in Law

Proof of Theorem 6. The functions $\mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y}) \rightarrow \mathbb{R}$ given by $\mu \mapsto \langle \psi, \mu \rangle$ for $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$ separate $\mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y})$ and form a set closed under addition. By Jakubowski [10, Theorem 4.6] the relative compactness of the laws of the processes $\langle \psi, \mu_t^n \rangle$, which was shown in Proposition 26, and the compact containment shown in Proposition 32 together establish relative compactness of the laws of the μ^n on $\mathbb{D}(\mathbb{R}_0^+, \mathcal{M}(\overline{\mathcal{X}} \times \mathcal{Y}))$. □

In constructing the processes μ_t^n no assumptions were made about the underlying probability spaces and Theorem 6 deals only with the laws of the processes. This allows any dependence (or independence) structure between the processes for different n . However, it is possible [4, Chapter 3, Theorem 1.8] or [11, Theorem 4.30] to sacrifice this freedom and choose a common probability space on which convergence occurs almost surely.

4 Properties of the Limit Points

First of all a number of auxiliary results are established in order to justify the reordering of various limiting operations needed when characterising the limit points.

Proposition 33. *Any limit point μ_t is continuous as a function of t , as is $\langle \psi, \mu_t \rangle$ for all $\psi \in C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y})$.*

Proof. The result is established for $\langle \psi, \mu_t \rangle$, the extension to μ_t is immediate, because the $\psi \in C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y})$ generate the topology on $\mathcal{M}(\bar{\mathcal{X}} \times \mathcal{Y})$.

Note that

$$\mathbb{P} \left(\sup_{s \leq t} |\langle \psi, \mu_s^n \rangle - \langle \psi, \mu_{s-}^n \rangle| > \frac{3 \|\psi\|}{n} \right) = 0 \quad (57)$$

and apply [4, Chapter 3, Theorem 10.2]. \square

Proposition 34. *For all $t \geq 0$ and $\psi \in C^{1,0}(\bar{\mathcal{X}} \times \mathcal{Y})$ there exists $A_{16}(t, \psi) \in \mathbb{R}^+$, independent of n such that*

$$\mathbb{E} \left[\frac{1}{n} \sup_{s \leq t} \left| \int_0^s \tilde{\mathcal{K}}_n \psi(X_n, r) dr \right| \right] \leq \frac{A_{16}(t, \psi)}{n}.$$

Proof. The following series of inequalities holds almost surely:

$$\begin{aligned} & \left| \int_0^s \tilde{\mathcal{K}}_n \psi(X_n, r) dr \right| \\ &= \left| \frac{1}{2n} \int_0^s \sum_{i=1}^{N_n(X_n(r))} [[K, \psi]](X_n(r, i), X_n(r, i)) dr \right| \\ &\leq \frac{3 \|\psi\|}{2n} K_\infty \int_0^s N_n(X_n(r)) dr \\ &\leq \frac{3 \|\psi\|}{2n} K_\infty s \sup_{r \leq s} N_n(X_n(r)). \quad (58) \end{aligned}$$

Now apply Proposition 15. \square

In the following it is assumed that the processes for different values of n are all defined on a joint probability space. One such space is discussed in §3.4, but here there is no requirement for almost sure convergence and a simple product space is sufficient.

Proposition 35. *For all $t \geq 0$*

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s^n(\bar{\mathcal{X}} \times \mathcal{Y}) \leq A_{10}(t) \text{ ult.} \right) = 1, \quad (59)$$

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s(\bar{\mathcal{X}} \times \mathcal{Y}) \leq A_{10}(t) \right) = 1 \quad (60)$$

and thus also

$$\mathbb{P} \left(\sup_{s \leq t} |\langle u \nabla \psi, \mu_s^n \rangle| \leq \|u\| \|\nabla \psi\| A_{10}(t) \text{ ult.} \right) = 1, \quad (61)$$

$$\mathbb{P} \left(\sup_{s \leq t} |\langle u \nabla \psi, \mu_s \rangle| \leq \|u\| \|\nabla \psi\| A_{10}(t) \right) = 1 \quad (62)$$

and

$$\mathbb{P} \left(\sup_{s \leq t} |\langle [K, \psi], \mu_s^n \otimes \mu_s^n \rangle| \leq 3K_\infty \|\psi\| A_{10}(t)^2 \text{ ult.} \right) = 1, \quad (63)$$

$$\mathbb{P} \left(\sup_{s \leq t} |\langle [K, \psi], \mu_s \otimes \mu_s \rangle| \leq 3K_\infty \|\psi\| A_{10}(t)^2 \right) = 1. \quad (64)$$

Proof. Equation (59) is the second statement of Proposition 16 and (61)&(63) follow immediately. To derive (60),(62)&(64) from the versions involving n , use Proposition 33 to see that μ_s is continuous in s and note that $\sup_{s \leq t}$ is continuous in the neighbourhood of continuous paths in Skorohod space. \square

Proposition 36. For every $t \geq 0$ and $x \in \mathcal{X}$

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s(\{x\} \times \mathcal{Y}) = 0 \right) = 1.$$

Proof. Let $B(x, \epsilon)$ be the open ϵ -ball around $x \in \mathcal{X} = [0, L]$ and write $u_{-\infty}$ for $\inf_{x \in \mathcal{X}} u(x)$

$$\begin{aligned} & \mathbb{P} \left(\sup_{s \leq t} \mu_s^n(B(x, \epsilon) \times \mathcal{Y}) > \frac{2e\epsilon t I(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + 2c_0\epsilon\epsilon \right) \\ &= \mathbb{P} \left(\sup_{s \leq t} \sum_{i=1}^{N(X_n(s))} \mathbf{1}_{B(x, \epsilon) \times \mathcal{Y}}(X_n(s, i)) > \frac{2e\epsilon t I(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + 2c_0\epsilon n\epsilon \right). \end{aligned} \quad (65)$$

Noting that the particles present at time 0 and with positions in $B(x, \epsilon)$ at some later time are stochastically dominated by a Poisson random variable with mean $2c_0\epsilon n\epsilon$ and the number incepted at later times is stochastically dominated by a Poisson random variable with mean $2c_0\epsilon n t I(\mathcal{X} \times \mathcal{Y})\epsilon / \inf_{x \in \mathcal{X}} u(x)$. Thus using Proposition 43 twice

$$\begin{aligned} & \mathbb{P} \left(\sup_{s \leq t} \mu_s^n(B(x, \epsilon) \times \mathcal{Y}) > \frac{2e\epsilon t I(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + 2c_0\epsilon\epsilon \right) \\ & \leq 2e^{-2n\epsilon t I(\mathcal{X} \times \mathcal{Y})/u_{-\infty}} + 2e^{-2c_0n\epsilon} \end{aligned} \quad (66)$$

and, by Borel-Cantelli, one sees

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s^n(B(x, \epsilon) \times \mathcal{Y}) \leq \frac{2e\epsilon t I(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + 2c_0\epsilon\epsilon \text{ ult.} \right) = 1. \quad (67)$$

By the continuity of the limit points μ_t (or the Portmanteau theorem)

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s(B(x, \epsilon) \times \mathcal{Y}) \leq 2e\epsilon \left(\frac{t I(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + c_0 \right) \right) = 1 \quad (68)$$

and

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s(\{x\} \times \mathcal{Y}) \leq 2e\epsilon \left(\frac{tI(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + c_0 \right) \right) = 1. \quad (69)$$

This holds for each $\epsilon > 0$. \square

Proposition 37. *Let $\mathcal{X}' = \{j\Delta x : j = 0, \dots, J\}$, which is the set of discontinuity points for the coagulation operators, then, for all $t \geq 0$*

$$\mathbb{P} \left(\sup_{s \leq t} \mu_s(\mathcal{X}' \times \mathcal{Y}) = 0 \right) = 1.$$

Proof. Since \mathcal{X}' is finite, apply Proposition 36. \square

Proposition 38. *For all $t \geq 0$*

$$\mathbb{P} \left(\lim_{n \rightarrow \infty} \langle [K, \psi], \mu_t^n \otimes \mu_t^n \rangle = \langle [K, \psi], \mu_t \otimes \mu_t \rangle \right) = 1,$$

where, for any measurable $B_1, B_2 \subset \overline{\mathcal{X}} \times \mathcal{Y}$, $\mu_t^n \otimes \mu_t^n(B_1 \times B_2) = \mu_t^n(B_1)\mu_t^n(B_2)$.

Proof. It is immediate that weak convergence of μ_t^n to μ_t implies weak convergence of $\mu_t^n \otimes \mu_t^n$ to $\mu_t \otimes \mu_t$ and Proposition 37 shows that the discontinuity set of $[K, \psi]$ has measure 0 under $\mu_t \otimes \mu_t$. \square

4.1 Weak Limit Equation

It is now possible to develop a weak limit equation for $\psi \in C^{1,0}(\overline{\mathcal{X}} \times \mathcal{Y})$ that also satisfy the boundary condition

$$\psi|_{\{L\} \times \mathcal{Y}} \equiv 0. \quad (70)$$

Using this boundary condition (39) simplifies to

$$\begin{aligned} \langle \psi, \mu_t^n \rangle &= \langle \psi, \mu_0^n \rangle + \int_0^t \langle u \nabla \psi, \mu_s^n \rangle ds + t \langle \psi, I \rangle \\ &\quad + \frac{1}{2} \int_0^t \langle [K, \psi], \mu_s^n \otimes \mu_s^n \rangle ds - \frac{1}{2n} \int_0^t \langle [[K, \psi]], \mu_s^n \rangle ds + M_n^\psi(t). \end{aligned} \quad (71)$$

The last two terms on the right hand side of (71) vanish with probability 1 as $n \rightarrow \infty$, by Proposition 34 and Proposition 20 respectively leaving

$$\begin{aligned} \lim_{n \rightarrow \infty} \langle \psi, \mu_t^n \rangle &= \lim_{n \rightarrow \infty} \langle \psi, \mu_0^n \rangle + \lim_{n \rightarrow \infty} \int_0^t \langle u \nabla \psi, \mu_s^n \rangle ds + t \langle \psi, I \rangle \\ &\quad + \lim_{n \rightarrow \infty} \frac{1}{2} \int_0^t \langle [K, \psi], \mu_s^n \otimes \mu_s^n \rangle ds. \end{aligned} \quad (72)$$

Proof of Theorem 7. As noted in §3.4 one can choose a probability space such that the processes μ^n converge almost surely to μ in $\mathbb{D}(\mathbb{R}_0^+, \mathcal{M}(\bar{\mathcal{X}} \times \mathcal{Y}))$. Continuity of the μ means this implies almost sure convergence in $\mathcal{M}(\bar{\mathcal{X}} \times \mathcal{Y})$ (which has the weak topology) for μ_t^n at any specified t . Thus, with probability 1,

$$\lim_{n \rightarrow \infty} \langle \psi, \mu_t^n \rangle = \langle \psi, \mu_t \rangle, \quad (73)$$

which deals with the first two terms in (72).

Regarding $\langle u \nabla \psi, \mu_s^n \rangle$ as a function of s , Proposition 35 allows the application of dominated convergence to show that, with probability 1,

$$\lim_{n \rightarrow \infty} \int_0^t \langle u \nabla \psi, \mu_s^n \rangle ds = \int_0^t \lim_{n \rightarrow \infty} \langle u \nabla \psi, \mu_s^n \rangle ds. \quad (74)$$

Since $u \nabla \psi$ is a bounded continuous function on $\bar{\mathcal{X}} \times \mathcal{Y}$, weak convergence shows that the pointwise (in time) limit of $\langle u \nabla \psi, \mu_t^n \rangle$ is $\langle u \nabla \psi, \mu_t \rangle$ and thus

$$\lim_{n \rightarrow \infty} \int_0^t \langle u \nabla \psi, \mu_s^n \rangle ds = \int_0^t \langle u \nabla \psi, \mu_s \rangle ds \quad \text{a.s.} \quad (75)$$

The same argument, with the addition of Proposition 38 for the final stage, shows that

$$\lim_{n \rightarrow \infty} \int_0^t \langle [K, \psi], \mu_s^n \otimes \mu_s^n \rangle ds = \int_0^t \langle [K, \psi], \mu_s \otimes \mu_s \rangle ds \quad \text{a.s.} \quad (76)$$

Collecting the terms together in the notation used here (note the theorem is stated using slightly more explicit, less compact notation)

$$\begin{aligned} \langle \psi, \mu_t \rangle &= \langle \psi, \mu_0 \rangle \\ &+ \int_0^t \langle u \nabla \psi, \mu_s \rangle ds + t \langle \psi, I \rangle + \frac{1}{2} \int_0^t \langle [K, \psi], \mu_s \otimes \mu_s \rangle ds. \end{aligned} \quad (77)$$

Since

$$\sup_{s \leq t} |\langle [K, \psi], \mu_s^n \rangle| \leq \frac{3 \|\psi\| K_\infty}{\Delta x} \sup_{s \leq t} \mu_s^n(\mathcal{X} \times \mathcal{Y}) \quad (78)$$

the expectation of the penultimate term in (71), which is the systematic error, is $\mathcal{O}(1/n)$. The zero mean martingale term is $\mathcal{O}(1/\sqrt{n})$ by Proposition 20.

□

4.2 Density

Proposition 39. *Assuming the μ^n are defined on a common probability space and without any restrictions on the presence or absence of a dependence structure then, for every $t \geq 0$ and $\delta > 0$*

$$\mathbb{P} \left(\sup_{x \in \bar{\mathcal{X}}} \sup_{s \leq t} \mu_s(\{x\} \times \mathcal{Y}) \geq \delta \right) = 0. \quad (79)$$

Proof. Choose $\epsilon \in \mathbb{R}^+$ such that

$$\epsilon < \frac{\delta}{2e} \left(\frac{tI(\mathcal{X} \times \mathcal{Y})}{u_{-\infty}} + c_0 \right)^{-1}. \quad (80)$$

One can cover $\overline{\mathcal{X}}$ with no more than $3L/\epsilon$ balls of radius ϵ . Let the centres of these balls be x_1, \dots, x_C , where C is the smallest integer not less than $3L/\epsilon$, thus

$$\mathbb{P} \left(\sup_{x \in \overline{\mathcal{X}}} \sup_{s \leq t} \mu_s(\{x\} \times \mathcal{Y}) \geq \delta \right) \leq \sum_{i=1}^C \mathbb{P}(\mu_t(B(x_i, \epsilon) \times \mathcal{Y}) \geq \delta) \quad (81)$$

and this is 0 by (68) in the proof of Proposition 36. \square

Proof of Theorem 8. For any measurable $B \subset \mathcal{Y}$ define a measure $\bar{\mu}_{t,B}$ on $\overline{\mathcal{X}}$ by $\bar{\mu}_{t,B}(A) = \mu_t(A \times B)$. By Proposition 39 this measure has no atoms and therefore a density with respect to Lebesgue measure. \square

It is thus possible to write $\mu_t(dx, dy)$ as $f(x; t, \mathcal{Y})dx\bar{\mu}_{t,\mathcal{Y}}(dy)$ with dx being Lebesgue measure on \mathcal{X} . Differentiability (with respect to x) remains an open problem. A true density would require the specification of a measure on the particle type space \mathcal{Y} against which the density could be integrated and which would then have to be related to the inception and coagulation processes. In general the attraction of stochastic particle based methods is that they place minimal restrictions on \mathcal{Y} and so \mathcal{Y} -densities are only to be expected in special cases. One very important such special case is when \mathcal{Y} is a discrete set and dy the counting measure, here the existence of a density such that $\mu_t(dx, dy) = c(t, x, y)dx dy$ is immediate.

Proof of Theorem 9. Substituting the definition of $[K, \psi]$ from (21) and the assumed density into (77) yields

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) c(t, x, y) dx dy = & \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) \nabla (u(x) c(t, x, y)) dx dy + \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) I(dx, dy) \\ & + \frac{1}{2} \sum_{j=1}^J \int_{(\mathcal{X}_j \times \mathcal{Y})^2} [\psi(x_1 + x_2, y_1) - \psi(x_1, y_1) - \psi(x_2, y_2)] \\ & \frac{K(x_1, y_2, x_2, y_2)}{\Delta x} c(t, x_1, y_1) dx_1 dy_1 c(t, x_2, y_2) dx_2 dy_2, \quad (82) \end{aligned}$$

where it is emphasised that the derivative only applies to the position variable, that is, the coordinate in \mathcal{X} . Substituting the assumed densities for the inception measure (I_{int} on $\mathcal{X}^\circ \times \mathcal{Y}$, the interior of the space and an inflow boundary component I_{bdry} on $\{0\} \times \mathcal{Y}$, which would be

singular with respect to Lebesgue measure on the whole space) one sees

$$\begin{aligned}
\frac{d}{dt} \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) c(t, x_1, x_2) dx_1 dx_2 = & \\
& - \int_{\mathcal{X}} u(0) \psi(0, y) c(t, 0, y) dy - \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) \nabla (u(x) c(t, x, y)) dx dy \\
& + \int_{\mathcal{X} \times \mathcal{Y}} \psi(x, y) I_{\text{int}}(x, y) dx dy + \int_{\mathcal{Y}} \psi(0, y) I_{\text{bdry}}(y) dy \\
& + \frac{1}{2} \sum_{j=1}^J \int_{(\mathcal{X}_j \times \mathcal{Y})^2} [\psi(x_1, y_1 + y_2) - \psi(x_1, y_1) - \psi(x_2, y_2)] \\
& \quad \frac{K(x_1, y_1, x_2, y_2)}{\Delta x} c(t, x_1, y_1) dx_1 dy_1 c(t, x_2, y_2) dx_2 dy_2, \quad (83)
\end{aligned}$$

using integration by parts (Gauss' theorem) and (70). Now restricting to test functions of the form $\psi(x, y) = \psi_1(x) \psi_2(y)$ for ψ_1 with a continuous bounded derivative, ψ_2 bounded and exploiting the fact that dy is counting measure on \mathcal{Y} and the symmetry of K , (83) holding for all ψ is equivalent to the following equation holding for all y and ψ_1 :

$$\begin{aligned}
\frac{d}{dt} \int_{\mathcal{X}} \psi_1(x) c(t, x_1, y) dx_1 = & \\
& - u(0) \psi_1(0) c(t, 0, y) - \int_{\mathcal{X}} \psi_1(x) \nabla (u(x) c(t, x, y)) dx \\
& + \int_{\mathcal{X}} \psi_1(x) I_{\text{int}}(x, y) dx + \psi_1(0) I_{\text{bdry}}(y) \\
& + \frac{1}{2} \sum_{j=1}^J \int_{\mathcal{X}_j^2} \psi_1(x_1) \sum_{\substack{y_1, y_2 \in \mathcal{Y} \\ y_1 + y_2 = y}} \frac{K(x_1, y_1, x_2, y_2)}{\Delta x} c(t, x_1, y_1) dx_1 c(t, x_2, y_2) dx_2 \\
& - \sum_{j=1}^J \int_{\mathcal{X}_j^2} \psi_1(x_1) c(t, x_1, y) \sum_{y_2 \in \mathcal{Y}} \frac{K(x_1, y, x_2, y_2)}{\Delta x} dx_1 c(t, x_2, y_2) dx_2. \quad (84)
\end{aligned}$$

To recover a partial differential equation for the density c , which is assumed differentiable in the \mathcal{X} -direction, let ψ_1 be a delta function located at an interior point of $\mathcal{X} \times \mathcal{Y}$ (strictly, a sequence of ψ_1 approximating such a delta function):

$$\begin{aligned}
\frac{\partial}{\partial t} c(t, x, y) = & - \nabla (u(x) c(t, x, y)) + I_{\text{int}}(x, y) \\
& + \frac{1}{2} \sum_{j=1}^J \mathbb{1}_{\mathcal{X}_j}(x) \sum_{\substack{y_1, y_2 \in \mathcal{Y} \\ y_1 + y_2 = y}} c(t, x, y_1) \int_{\mathcal{X}_j} \frac{dx_2}{\Delta x} K(x, y_1, x_2, y_2) c(t, x_2, y_2) \\
& - c(t, x, y) \sum_{j=1}^J \mathbb{1}_{\mathcal{X}_j}(x) \sum_{y_2 \in \mathcal{Y}} \int_{\mathcal{X}_j} \frac{dx_2}{\Delta x} K(x, y, x_2, y_2) c(t, x_2, y_2) \quad (85)
\end{aligned}$$

An inflow boundary condition can be recovered by taking $\psi_1(x)$ approximating

$$\mathbb{1}_{\{0\}}(x) \tag{86}$$

to get

$$0 = -u(0)c(t, 0, y_1) + I_{\text{bdry}}(y_1). \tag{87}$$

No boundary condition is to be expected on $\{L\} \times \mathcal{Y}$ for a first order advection problem. In any case, it is not possible to extract one using the method above because of the requirement that ψ be 0 on this boundary.

□

5 Conclusion

The convergence of stochastic particle systems representing physical advection, inflow, outflow and coagulation has been demonstrated. The problem was studied on a bounded spatial domain such that there was a general upper bound on the residence time of a particle. The laws on the appropriate Skorohod path space of the empirical measures of the particle systems were shown to be relatively compact. The paths charged by the limits were characterised as solutions of a weak equation, but only for functions taking the value zero on the outflow boundary. The limit points of the empirical measures were shown to have densities with respect to Lebesgue measure when projected on to physical position space. In the case of a discrete particle type space a strong form of the Smoluchowski coagulation equation with a delocalised coagulation interaction and an inflow boundary condition was derived. As the spatial discretisation is refined in the limit equations, the delocalised coagulation term reduces to the standard local Smoluchowski interaction.

The analysis presented in this paper focuses on particle systems of the direct simulation type. The extension to weighted particle [18] methods introduces various complications because the coagulation operators are no longer bounded. Similar problems would arise when extending the results presented here to the additive coagulation kernel and should be treatable by imposing sufficient conditions on the inception rate so that coagulation can be tightly controlled by controlling the material available for coagulation.

5.1 Acknowledgements

The author is indebted to Wolfgang Wagner for his patient advice and for drawing his attention to a copy of Davis [1], from which the present work started. He also thanks Sabine Jansen for some helpful explanations.

A Jump Kernel

The properties of the jump kernel are essential in order to justify the application of [1, Theorem 25.5] during the proof of Theorem 5 at the end of §2.2

Definition 40. Let \mathcal{E} be the Borel σ -algebra on E , $A \in \mathcal{E}$, and define $Q_n : \bar{E} \times \mathcal{E} \rightarrow \mathbb{R}_0^+$ by

$$Q_n(X, A) := (Q_n^{\text{in}}(X, A) + Q_n^{\text{coag}}(X, A)) \frac{\mathbb{1}(X \in E)}{\lambda_n(X)} + \mathbb{1}_A(J^{\text{exit}}(X)) \mathbb{1}(X \in \bar{E} \setminus E).$$

where J^{exit} is the jump that results from removing all particles with position L , that is, in $\bar{\mathcal{X}} \setminus \mathcal{X}$,

$$Q_n^{\text{in}}(X, A) := nI(A)$$

and

$$Q_n^{\text{coag}}(X, A) := \sum_{j=1}^J \sum_{\substack{N(X) \\ i_1, i_2=1 \\ i_1 \neq i_2}} K(X(i_1), X(i_2)) \mathbb{1}_{\mathcal{X}_j}(X(i_1, 1)) \mathbb{1}_{\mathcal{X}_j}(X(i_2, 1)) \mathbb{1}_A(J^{\text{coag}}(i_1, i_2, X))$$

with J^{coag} being the coagulation jump defined in §2.1.3.

Proposition 41. Q_n is a probability kernel from \bar{E} to E and $Q_n(X, \{X\}) = 0$ for all $X \in E$.

Proof. Note first that $Q_n^{\text{in}}(X, E) + Q_n^{\text{coag}}(X, E) = \lambda_n(X) \forall X \in E$ so that, if Q is a kernel, it is certainly a probability kernel. By [11, Lemma 1.40] it is sufficient to check that $X \mapsto Q_n(X, A)$ is measurable for each $A \in \mathcal{E}$. Q_n^{in} is trivially measurable in X . To see that Q_n^{coag} is measurable, note that J^{coag} is continuous in X .

For the measurability of J^{exit} , define \mathcal{S} from E to the power set of $\bar{E} \setminus E$ by

$$\mathcal{S}(X) := (\{L\} \times \mathcal{Y}) \cup \bigcup_{i=1}^{N(X)} \bigotimes_{i_1=1}^i \{X(i_1)\} \times (\{L\} \times \mathcal{Y}) \times \bigotimes_{i_1=i+1}^{N(X)} \{X(i_1)\}, \quad (88)$$

which maps measurable subsets of E onto measurable subsets of \bar{E} . Writing

$$J^{\text{exit}^{-1}}(A) = \bigcup_{i \in \mathbb{N}} \mathcal{S}^i(A) \quad (89)$$

shows the required measurability. □

B Auxiliary Results

All notation used in this appendix is defined here and is independent of the main text.

Proposition 42. *Let X_n be random variables such that $\mathbb{E}[X_n] = n\lambda$ for some $\lambda \in \mathbb{R}^+$, $\text{var}(X_n) \leq n\sigma^2$ for some $\sigma \in \mathbb{R}^+$ and $\epsilon \in \mathbb{R}^+$, then*

$$\mathbb{P}\left(\left|\frac{X_n - n\lambda}{n}\right| \geq \frac{\sigma}{\sqrt{\epsilon}}\right) \leq \frac{\epsilon}{n}.$$

Proof. Chebyshev's inequality. □

A particular application of this proposition is when $X_n \sim \text{Poi}(n\lambda)$ in which case one can take $\sigma^2 = \lambda$.

Proposition 43. *Let X_n be Poisson random variables such that $\mathbb{E}[X_n] = n\lambda$ for some $\lambda \in \mathbb{R}^+$, then*

$$\mathbb{P}\left(\frac{X_n - ne\lambda}{n} > 0\right) \leq 2e^{-n\lambda}.$$

Proof.

$$\begin{aligned} \mathbb{P}\left(\frac{X_n - ne\lambda}{n} > 0\right) &= \sum_{i=[ne\lambda]}^{\infty} \frac{e^{-n\lambda}(n\lambda)^i}{i!} \\ &\leq \frac{e^{-n\lambda}(n\lambda)^{[ne\lambda]}}{[ne\lambda]!} \sum_{i=0}^{\infty} \frac{(n\lambda)^i [ne\lambda]!}{[ne\lambda + i]!} \leq \frac{e^{-n\lambda}(n\lambda)^{[ne\lambda]}}{[ne\lambda]!} \sum_{i=0}^{\infty} \left(\frac{n\lambda}{ne\lambda}\right)^i. \end{aligned}$$

Noting that $\sum e^{-i} \leq \sum 2^{-i} = 2$ and $n^n e^{-n} \leq n!$, one has

$$\begin{aligned} \mathbb{P}\left(\frac{X_n - ne\lambda}{n} > 0\right) &\leq 2 \frac{e^{-n\lambda}(n\lambda)^{[ne\lambda]}}{[ne\lambda]^{[ne\lambda]} e^{-[ne\lambda]}} \\ &\leq 2e^{ne\lambda - n\lambda} \left(\frac{n\lambda}{ne\lambda}\right)^{[ne\lambda]} \leq 2e^{-n\lambda}. \end{aligned}$$

□

Proposition 43 puts a much weaker bound on X_n than Proposition 42, but the exponential decay in the probability enables the application of Borel–Cantelli.

Proposition 44. *Let M_t be a locally square integrable Martingale with respect to a filtration $(\mathcal{F}_t)_{t \in \mathbb{R}_0^+}$ and T'_i an almost surely increasing sequence of stopping times such that $T'_i \rightarrow \infty$ a.s.. Let $t > 0$ and define $T''_i = T'_i \wedge t$. Then*

$$\mathbb{E}[(M_t - M_0)^2] = \sum_{i=1}^{\infty} \mathbb{E}\left[\left(M_{T''_i} - M_{T''_{i-1}}\right)^2\right] \quad (90)$$

Proof. Using the square integrability to show that all expectations exist and [11, Theorem 7.29] for the final step

$$\begin{aligned}
\mathbb{E} [(M_t - M_0)^2] &= \mathbb{E} [M_t^2] - \mathbb{E} [M_0^2] \\
&= \sum_{l=1}^{\infty} \mathbb{E} [M_{T_l''}^2 - M_{T_{l-1}''}^2] = \sum_{l=1}^{\infty} \mathbb{E} \left[\mathbb{E} [M_{T_l''}^2 - M_{T_{l-1}''}^2 \mid \mathcal{F}_{T_{l-1}''}] \right] \\
&= \sum_{l=1}^{\infty} \mathbb{E} \left[\mathbb{E} \left[\left(M_{T_l''} - M_{T_{l-1}''} \right)^2 + 2M_{T_l''}M_{T_{l-1}''} - 2M_{T_{l-1}''}^2 \mid \mathcal{F}_{T_{l-1}''} \right] \right] \\
&= \sum_{l=1}^{\infty} \mathbb{E} \left[\left(M_{T_l''} - M_{T_{l-1}''} \right)^2 \right] \quad (91)
\end{aligned}$$

□

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