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Convergence of the EBT method for a non-local model of cell proliferation with discontinuous interaction kernel

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We consider the EBT algorithm (a particle method) for the nonlocal equation with a discontinuous interaction kernel. The main difficulty lies in the low regularity of the kernel, which is not Lipschitz continuous, thus preventing the application of standard arguments. Therefore, we use the radial symmetry of the problem instead and transform it using spherical coordinates. The resulting equation has a Lipschitz kernel with only one singularity at zero. We introduce a new weighted flat norm and prove that the particle method converges in this norm. We also comment on the two-dimensional case that requires the application of the theory of measure spaces on general metric spaces and present numerical simulations confirming the theoretical results. In a companion paper we apply the Bayesian method to fit parameters to this model and study its theoretical properties.

Keywords: particle method; EBT algorithm; measure solutions; flat metric; nonlocal equation; convergence analysis; cancer modelling.

1. Introduction

In this paper we study a numerical algorithm to solve the nonlocal equation

$$\partial_t n(x,t) \;=\; k * n(x,t)\Big(1 \;-\; n(x,t)\Big), \tag{1.1}$$

where $k = \mathbb{1}_{B_\sigma(0)}/|B_\sigma(0)|$ is the so-called interaction kernel, $B_\sigma(0)$ denotes a ball centred at 0 with radius σ and volume $|B_\sigma(0)|$, while

$$k * n(x,t) \;=\; \int_{\mathbb{R}^d} k(x-y)\, n(y,t)\, \mathrm{d}y.$$

In what follows we focus on the case $d = 3$, but the case $d = 2$ is not completely abandoned and is discussed in Section 7.

Recently, we have proposed model (1.1) to describe cells' proliferation within a solid tumour, for which we used Bayesian methodology to estimate model parameters (Szymańska *et al.*, 2021a).

Although our modelling approach differs from those proposed earlier there are examples of other interesting models describing the dynamics of multicellular spheroids, like the ones proposed by Byrne & Chaplain (1995, 1996, 1998) studied in several analytical papers (Cui & Friedman, 2003; Chen *et al.*, 2005; Friedman & Hu & (2006a, 2006b)).

In the case, k is compactly supported and Lipschitz continuous, one can solve (1.1) using the classical particle method (de Roos 1988; Gwiazda *et al.* (2014, 2017); Carrillo *et al.* 2019), originally studied in the context of fluid dynamics and kinetic theory (Cottet & Raviart, 1984; Raviart, 1985; Ganguly & Victory, 1989; Goodman *et al.*, 1990; Westdickenberg & Wilkening, 2010; Chertock *et al.*, 2012; Duan & Liu, 2016; Gao & Liu, 2017) and brought to mathematical biology by de Roos (1988, 1997); de Roos & Persson (2001). This can be possibly combined with the splitting technique Colombo & Corli, (2004); Carrillo *et al.* (2014, 2018). In these algorithms one divides the population into smaller groups called cohorts. This allows transforming partial differential equation (1.1) to a system of ordinary differential equations (ODEs) for the masses of all cohorts. Localizations of cohorts are constant as there is no transport term in (1.1).

To prove numerical convergence of these methods, one embeds the problem into the space of nonnegative Radon measures, where each cohort is represented by a Dirac mass (Gwiazda *et al.*, 2010, 2016b; Gwiazda & Marciniak-Czochra, 2010; Carrillo *et al.*, 2012; Ulikowska, 2012; Evers *et al.* (2015, 2016)). The convergence above is shown with respect to the flat norm (bounded Lipschitz distance), whose main properties are reviewed in Section 2. One can also prove the convergence with respect to weak* topology on the space of measures (Chertock *et al.*, 2012; Brännström *et al.*, 2013), but this is formally a weaker result and it does not yield convergence estimate as weak* topology is not explicitly metrizable. Moreover, a simple variant of flat norm proved to be useful for optimal control problems in spaces of measures, which may result in the future application of particle methods for such problems (Gwiazda *et al.*, 2019; Ackleh *et al.*, 2020b; Skrzeczkowski, 2020).

We remark that particle methods have been used in the more general context of structured population models (with transport term) and we refer to (Düll *et al.*, 2021, Chapter 4) for the systematic treatment of this topic. Moreover, the flat norm in the spaces of measures can be used to prove convergence of other schemes, including higher-order finite difference schemes, see Ackleh *et al.* (2017, 2020a); Ackleh & Miller (2019). We also note that these methods are widely used in the community of theoretical biologists and ecologists, see for instance Falster *et al.* (2016; 2017); Zhang *et al.* (2017).

Recall that we deal with $k = \mathbb{1}_{B_\sigma(0)}/|B_\sigma(0)|$ so that k jumps at the boundary of $B_\sigma(0)$ and is not even continuous. However, one may use the radial symmetry of the problem to gain some regularity. After moving to spherical coordinates (1.1) takes the form

$$\partial_t p(R,t) \; = \; \Big(4\pi R^2 \; - \; p(R,t)\Big) \int_0^\infty L(R,r)\, p(r,t)\, \mathrm{d}r, \tag{1.2}$$

where $p(R,t) = 4\pi R^2\, n((0,0,R),t)$ and $L(R,r)$ is given by (3.2). It turns out that after appropriate modification of the flat norm one can apply the particle method. More precisely, we write

$$p(\cdot,t) \approx \sum_{i=1}^{N} m_i(t)\, \delta_{x_i}(\cdot), \qquad x_i = \frac{i}{N} R_0, \tag{1.3}$$

where δ_{x_i} denotes Dirac measure at x_i representing a particle, m_i is the mass concentrated at x_i while R_0 is some parameter restricting the domain of interest (in general, the equation enjoys infinite-speed-of-propagation property and the solution is not compactly supported). Inserting (1.3) into (1.2) yields formally system of ODEs for masses

$$\partial_t m_i(t) = \left(4\pi x_i^2 \frac{R_0}{N} - m_i(t)\right) \sum_{j=1}^{N} L(x_i, x_j)\, m_j(t), \tag{1.4}$$

where $m_i(0)$ are chosen so that $p(\cdot,0) \approx \sum_{i=1}^{N} m_i(0)\,\delta_{x_i}(\cdot)$. Equation (1.4) is solvable by some standard algorithms, for instance Euler or Runge–Kutta method.

The main result of this paper reads:

THEOREM 1.1 Let $p(r,0) = 4\pi r^2 n_0(r)$ where $n_0 : \mathbb{R}^+ \to \mathbb{R}^+$ is bounded and compactly supported. Consider approximation of $p(r,0)$ in the space of measures

$$\mu_0^N(\cdot) = \sum_{i=1}^{N} m_i(0)\,\delta_{x_i}(\cdot), \qquad m_i(0) = \int_{x_{i-1}}^{x_i} p(r,0)\,\mathrm{d}r.$$

Let $p(r,t)$ be the solution to (1.1) with initial condition $p(r,0)$ and $\mu_t^N = \sum_{i=1}^{N} m_i(t)\,\delta_{x_i}$, where $m_i(t)$ solve (1.4). Then, there is a constant C independent of $R_0 > 1$ and N such that

$$\left\| p(\cdot,t) - \mu_t^N \right\|_{BL^*,w} \le C\,\frac{R_0^2}{N} + C\,e^{-R_0}, \tag{1.5}$$

where the weighted norm $\|\cdot\|_{BL^*,w}$ is defined by (2.9) and $p(\cdot,t)$ is identified with the measure $p(\cdot,t)(A) = \int_A p(r,t)\,\mathrm{d}r$.

We remark that the term e^{-R_0} in the error estimate in Theorem 1.1 comes from the fact that the solution is supported on the whole line $\mathbb{R}^+$, even if the initial data are compactly supported. In other words this term represents error coming from the truncation of the support of the solution.

The first novelty of this paper concerns application of radial symmetry of the problem to gain sufficient regularity of the kernel. After the change of variables (see Section 3), using the weighted norm introduced in (2.9), we incorporate singularity at $R, r = 0$ into the definition of the norm. A crucial observation is the following inequality

$$\left|\partial_R L(R,r)\right| \le \frac{1}{R}\left(\frac{2\sigma\,\mathcal{C}_\sigma}{r} + L(R,r)\right),$$

where $\mathcal{C}_\sigma$ is the constant defined in (3.7). This inequality measures in a sufficiently optimal way the singularity of Lipschitz constant of L as $R, r \to 0$. The factors $\frac{1}{R}, \frac{1}{r}$ will be incorporated into the definition of the weighted flat norm, cf. (2.9).

Another novelty of this paper is related to the case $d = 2$. It is known that particle method convergence is related to the Lipschitz regularity of L, but for $d = 2$ we only know that (except $R, r = 0$) L is only 1/2-Hölder continuous, cf. (7.2). However, one may observe that if L is only 1/2-Hölder continuous with respect to the usual Euclidean metric, it is Lipschitz continuous with respect to the Hölder metric $d_{1/2} = |x-y|^{1/2}$. This results in a different order of convergence as discussed in estimates in Section 7. We refer the reader to the recent monograph (Düll *et al.*, 2021) presenting the theory of measure spaces on general metric spaces.

Let us comment the assumption about the radial symmetry of the initial condition and the kernel. It is indeed a limitation, but still, there remains a significant range of applicability of the model. It is indeed a limitation, but still, there remains a significant range of applicability of the model. MCTs closely mimic in vivo solid tumours' main features, such as structural organisation and the gradients of oxygen, pH, and nutrients (Han *et al.*, 2021). Moreover, from the point of view of our main goal, that assumption was necessary. Namely, the present manuscript is an analytical complement to our modelling paper in which we used the Bayesian method to estimate the parameters of the model (Szymańska *et al.*, 2021a). The Bayesian method is in turn based on the Markov Chain Monte Carlo method (precisely, in our approach, we use the Metropolis–Hasting algorithm). To acquire the ergodic properties of the Markov Chain we had to solve the model for each data set around 50 000 times, that is once at each step of the Metropolis–Hasting algorithm. Therefore, the transformation of the three-dimensional model to the one-dimensional radial problem was necessary for computational complexity reduction and enabled parameter estimation within a reasonable time. Importantly, the size of the mesh increases exponentially with the dimension. Therefore, excluding the assumption about the radial symmetry of the initial conditions, and performing the parameter estimation within the three-dimensional formulation, does not necessarily increase the range of applicability of the model, as we encounter significant difficulty in terms of computational complexity. Last but not the least, we remark that the result concerning the stability of the numerical method is essential for proving the stability of *a posteriori* distributions obtained in the Bayesian method (Franklin, 1970; Mandelbaum, 1984; Bennett & Budgell, 1987; Fitzpatrick, 1991; Stuart, 2010; Gwiazda *et al.*, 2016a; Dashti & Stuart, 2017).

One may also ask if the problem of irregularity of the kernel k is purely academic, as one can approximate the characteristic function by convolution, for instance with the density of Gaussian distribution $\mathcal{N}(0, \sigma^2)$. However, when one performs classical particle methods with such kernel, the resulting estimates will be of size $\frac{C}{\sigma^{d+1}}$ (as this is the Lipschitz constant of the density of the d-dimensional Gaussian distribution and so the Lipschitz constant of the convolution), i.e. the estimates will blow up as $\sigma \to 0$. In this sense our result has theoretical importance, as it shows that radial symmetry may be used to gain additional regularity, which allows obtaining estimates independent of irregularity of the kernel.

The structure of the paper is as follows. In Section 2 we review necessary concepts from measure theory including weighted flat norm. Then, in Section 3, we perform the radial change of variables and we study properties of the radial kernel $L(R, r)$. Section 4 is devoted to the well-posedness of the radial equation (1.2), including continuity estimates. In Section 5 we obtain estimates for (1.2) that allow us to neglect the effect of infinite speed of propagation, so we can assume the support of the solution to be bounded. Moreover, we show how to interpret solutions to the numerical scheme as measure solutions so that they can be compared with exact measure solutions. Finally, in Section 6, we prove the main convergence result. Section 7 discusses necessary changes to handle a two-dimensional case, while Section 8 is devoted to the presentation of numerical simulations confirming theoretical results.

2. Relevant measure theory

Let $\mathcal{M}(\mathbb{R}^+)$ be the space of bounded real-valued signed Borel measures on S, cf. (Folland, 1984, Sections 1.3, 3.1). Intuitively, if $\mu \in \mathcal{M}(\mathbb{R}^+)$, then μ assigns a real number to each measurable subset $A \subset S$, which is a measure of the subset $\mathbb{R}^+$. This generalizes distributions with densities in the sense that if μ has density $n(x)$, we have

$$\mu(A) = \int_A n(x)\,\mathrm{d}x.$$

We note that the space of measures is a vector space; in particular, the difference between two measures is again a measure. We also write $\mathcal{M}^+(\mathbb{R}^+)$ for the subset of non-negative measures on $\mathbb{R}^+$, i.e. when $\mu \in \mathcal{M}^+(\mathbb{R}^+)$, we have $\mu(A) \geq 0$ for all subsets $A \subset \mathbb{R}^+$. From the point of view of applications non-negative measures model biological quantities like size, age or spread of population.

Hahn–Jordan decomposition. We recall that if $\mu \in \mathcal{M}(\mathbb{R}^+)$ is the signed measure, then there are (uniquely determined) two non-negative measures $\mu^+, \mu^- \in \mathcal{M}^+(\mathbb{R}^+)$ with disjoint supports such that

$$\mu = \mu^+ - \mu^-.$$

We call (μ^+, μ^-) the Hahn–Jordan decomposition of μ.

Norms on the space of measures. To perform analysis in spaces of measures one needs to equip them with norms. Three meaningful choices will be exploited below: total variation, flat norm and weighted flat norm.

Total variation. If $\mu \in \mathcal{M}(\mathbb{R}^+)$ we define total variation of μ as

$$\|\mu\|_{TV} := \mu^+(\mathbb{R}^+) + \mu^-(\mathbb{R}^+), \tag{2.1}$$

where μ^+, μ^- is the Hahn–Jordan decomposition of μ.

Flat norm. The second choice is the flat norm (or bounded Lipschitz distance) defined as

$$\|\mu\|_{BL^*} := \sup\left\{\int_{\mathbb{R}^+} \psi\,\mathrm{d}\mu : \psi \in BL(\mathbb{R}^+), \|\psi\|_{BL} \leq 1\right\}, \tag{2.2}$$

where the space of bounded Lipschitz functions $BL(\mathbb{R}^+)$ is given by

$$BL(\mathbb{R}^+) = \left\{f : \mathbb{R}^+ \to \mathbb{R} \text{ is continuous and } \|f\|_\infty < \infty, |f|_{Lip} < \infty\right\}, \tag{2.3}$$

where

$$\|f\|_\infty = \sup_{x\in\mathbb{R}^+} |f(x)|, \qquad |f|_{Lip} = \sup_{x\neq y} \frac{|f(x) - f(y)|}{|x-y|}. \tag{2.4}$$

Space $BL(\mathbb{R}^+)$ is equipped with the norm

$$\|f\|_{BL} = \max\Big(\|f\|_\infty, |f|_{Lip}\Big) \leq \|f\|_\infty + |f|_{Lip}. \tag{2.5}$$

Bounded Lipschitz distance in the space of measures has been used frequently in recent years, for instance, to study structured population models (Carrillo *et al.*, 2012), numerical algorithms (Carrillo *et al.*, 2014, 2019) or segregation in cross-diffusion systems (Carrillo *et al.*, 2018).

Now, we list some simple properties that are helpful when one works in the flat norm setting. For the proof see Remark 1.23, Proposition 1.44 and Theorem C.2 in Düll *et al.*, 2021 as well as (Evans, 2010, Theorems 4, 6; Section 5.8).

LEMMA 2.1 Let $f, g \in BL(\mathbb{R}^+)$ and $\mu \in \mathcal{M}(\mathbb{R}^+)$.

(A) We have $\left|\int_{\mathbb{R}^+} f(x)\, \mathrm{d}\mu(x)\right| \leq \|f\|_{BL} \|\mu\|_{BL^*}$.

(A') If $h \in L^\infty(\mathbb{R}^+)$ then $\left|\int_{\mathbb{R}^+} h(x)\, \mathrm{d}\mu(x)\right| \leq \|h\|_\infty \|\mu\|_{TV}$.

(B) If additionally $\mu \in \mathcal{M}^+(\mathbb{R}^+)$ then $\|\mu\|_{TV} = \|\mu\|_{BL^*}$.

(C) We have $f\, g \in BL(\mathbb{R}^+)$ and $\|f\, g\|_{BL} \leq 2\, \|f\|_{BL} \|g\|_{BL}$.

(D) (Rademacher's theorem) $f \in BL(\mathbb{R}^+)$ if and only if $f \in W^{1,\infty}(\mathbb{R}^+)$, i.e. $f, f' \in L^\infty(\mathbb{R}^+)$. Moreover,

$$|f|_{Lip} \leq \|f'\|_\infty.$$

Sketch of the proof. For (A) we note that $f/\|f\|_{BL}$ is bounded by 1 in $BL(\mathbb{R}^+)$ so that by (2.2) $\left|\int_{\mathbb{R}^+} \frac{f(x)}{\|f\|_{BL}}\, \mathrm{d}\mu(x)\right| \leq \|\mu\|_{BL^*}$. For (B) we note that we always have $\|\mu\|_{TV} \geq \|\mu\|_{BL^*}$ and the opposite inequality follows by choosing $\psi(r) = 1$ in (2.2) (this uses $\mu \in \mathcal{M}^+(\mathbb{R}^+)$). For (C) we observe that $\|f\, g\|_\infty \leq \|f\|_\infty \|g\|_\infty \leq \|f\|_{BL} \|g\|_{BL}$. Moreover, for $x, y \in \mathbb{R}^+$, we have

$$|f(x)\, g(x) - f(y)\, g(y)| \leq \left(\|f\|_\infty |g|_{Lip} + \|g\|_\infty |f|_{Lip}\right) |x - y| \leq 2\|f\|_{BL} \|g\|_{BL} |x - y|$$

so that $|f\, g|_{Lip} \leq 2\|f\|_{BL} \|g\|_{BL}$. Hence, (C) follows. For (D) see (Evans, 2010, Theorems 4, 6; Section 5.8). □

Weighted flat norm. This is the analogue of the flat norm applicable for singular problems like in this paper. First, we define weighted measure μ/f. Given a non-negative measurable function $f : \mathbb{R}^+ \to \mathbb{R}^+$ and a non-negative measure $\mu \in \mathcal{M}^+(\mathbb{R}^+)$, we define measure μ/f with

$$\frac{\mu}{f}(A) = \int_A \frac{1}{f(r)}\, \mathrm{d}\mu(r). \tag{2.6}$$

This equality defines measure (possibly not finite). Now, we extend this definition to $\mu \in \mathcal{M}(\mathbb{R}^+)$. Let μ^+, μ^- be Hahn–Jordan decomposition of μ. If $\frac{\mu^+}{f}, \frac{\mu^-}{f}$ are finite measures, we define

$$\frac{\mu}{f}(A) = \frac{\mu^+}{f}(A) - \frac{\mu^-}{f}(A). \tag{2.7}$$

By non-negativity of f and uniqueness of Hahn–Jordan decomposition, we have

$$\left\|\frac{\mu}{f}\right\|_{TV} = \left\|\frac{\mu^+}{f}\right\|_{TV} + \left\|\frac{\mu^-}{f}\right\|_{TV}.$$

It follows that if $\frac{\mu^+}{f}$, $\frac{\mu^-}{f}$ are finite measures then $\left\|\frac{\mu}{f}\right\|_{TV} < \infty$. Whenever this is true, it makes sense to write $\left\|\frac{\mu}{f}\right\|_{BL^*}$, which is the weighted flat norm of μ with weight f.

The most important case is $f(r) = r$. We define

$$\mathcal{M}_w(\mathbb{R}^+) := \left\{\mu \in \mathcal{M}(\mathbb{R}^+) : \left\|\frac{\mu^+}{r}\right\|_{TV}, \left\|\frac{\mu^-}{r}\right\|_{TV} < \infty\right\}. \tag{2.8}$$

We also write $\mathcal{M}_w^+(\mathbb{R}^+)$ for the subspace of non-negative measures in $\mathcal{M}_w(\mathbb{R}^+)$. The idea is that $\mathcal{M}_w(\mathbb{R}^+)$ consists of measures that vanish at least linearly at $r = 0$. For $\mu \in \mathcal{M}_w(\mathbb{R}^+)$, we define

$$\|\mu\|_{BL^*,w} := \sup\left\{\int_{\mathbb{R}^+} \frac{\psi(r)}{r}\, \mathrm{d}\mu(r) : \psi \in BL(\mathbb{R}^+), \|\psi\|_{BL} \le 1\right\}. \tag{2.9}$$

We conclude with one of the most useful properties of the flat norm.

Lemma 2.2 Space $(\mathcal{M}_w^+(\mathbb{R}^+), \|\cdot\|_{BL^*,w})$ is a complete metric space.

Proof. Let $\{\mu_n\}_{n\in\mathbb{N}}$ be a Cauchy sequence in $(\mathcal{M}_w^+(\mathbb{R}^+), \|\cdot\|_{BL^*,w})$. Let $\nu_n = \mu_n/r$. Then, $\{\nu_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence in $(\mathcal{M}(\mathbb{R}^+), \|\cdot\|_{BL^*})$. As $(\mathcal{M}^+(\mathbb{R}^+), \|\cdot\|_{BL^*})$ (Düll *et al.*, 2021, Theorem 1.61) or (Gwiazda *et al.*, 2010, Theorem 2.7 (ii)) $\nu_n \to \nu$ in $(\mathcal{M}^+(\mathbb{R}^+), \|\cdot\|_{BL^*})$. Let $\mu = r\,\nu$. Then, $\mu \in \mathcal{M}_w^+(\mathbb{R}^+)$. We claim that $\mu_n \to \mu$ in $(\mathcal{M}_w^+(\mathbb{R}^+), \|\cdot\|_{BL^*,w})$. Indeed, for all $\psi \in BL(\mathbb{R}^+)$ with $\|\psi\|_{BL} \le 1$, we have

$$\int_{\mathbb{R}^+} \frac{\psi(r)}{r}\, \mathrm{d}(\mu_n - \mu)(r) = \int_{\mathbb{R}^+} \psi(r)\, \mathrm{d}(\nu_n - \nu)(r) \le \|\nu_n - \nu\|_{BL^*}.$$

Taking supremum over the left-hand side, we get

$$\|\mu_n - \mu\|_{BL^*,w} \le \|\nu_n - \nu\|_{BL^*} \to 0.$$

□

The most important property of the flat norm is that in the topology generated by the flat norm, any measure can be approximated with an appropriate combination of Dirac masses.

Lemma 2.3 Let $\mu \in \mathcal{M}^+[0, R_0]$ and $f : \mathbb{R}^+ \to \mathbb{R}^+$ be such that $\left\|\frac{\mu}{f}\right\|_{TV} = \int_{[0,R_0]} \frac{1}{f(r)}\, \mathrm{d}\mu(r) < \infty$. Consider $\mu^N = \sum_{k=1}^N \mu(A_k^N)\, \delta_{x_k^N}$ with $x_k^N = \frac{k}{N} R_0$ and

$$A_k^N = \left[\frac{k-1}{N} R_0, \frac{k}{N} R_0\right) \subset \mathbb{R} \text{ for } k = 1, ..., N-1 \quad \text{and} \quad A_N^N = \left[\frac{N-1}{N} R_0, R_0\right] \subset \mathbb{R}.$$

Then,

$$\left\| \frac{\mu^N - \mu}{f} \right\|_{BL^*[0,R_0]} \leq \frac{R_0}{N} \left\| \frac{\mu}{f} \right\|_{TV}.$$

Proof. Directly from the definition, we obtain

$$\left\| \frac{\mu^N - \mu}{f} \right\|_{BL^*[0,R_0]} = \sup_{\psi} \int_{[0,R_0]} \frac{\psi(r)}{f(r)} \,\mathrm{d}(\mu^N - \mu)(r) = \sup_{\psi} \sum_{k=1}^{N} \int_{A_k^N} \frac{\left(\psi(x_k^N) - \psi(r)\right)}{f(r)} \,\mathrm{d}\mu(r),$$

where the supremum is taken above all $\psi \in BL[0,R_0]$ with $\|\psi\|_{BL} \leq 1$. As $\left|\psi(x_k^N) - \psi(r)\right| \leq \frac{R_0}{N}$ the proof is concluded. □

REMARK 2.4 The same proof as for Lemma 2.3 shows the following. Consider the usual Lebesgue measure λ on $[0,R_0]$. Let $\lambda^N = \frac{R_0}{N} \sum_{k=1}^{N} \delta_{x_k^N}$ with $x_k^N = \frac{k}{N} R_0$. Then,

$$\left\| \lambda^N - \lambda \right\|_{BL^*[0,R_0]} \leq \frac{R_0^2}{N}.$$

3. Radial change of variables

In this section we transform the original problem (1.1) using radial change of variables. Then, we study the basic properties of the resulting radial interaction kernel that are relevant for algorithm convergence.

THEOREM 3.1 (Radial change of coordinates). Let $n(x,t)$ be the solution to (1.1) with radially symmetric initial condition $n_0(x)$. Let the radial densities $p(R,t)$ and $p_0(R)$ be defined by

$$p(R,t) = 4\pi R^2\, n((0,0,R),t), \qquad p_0(R) = 4\pi R^2\, n_0((0,0,R)).$$

Then, the following equation is satisfied

$$\begin{aligned} \partial_t p(R,t) &= \left(4\pi R^2 - p(R,t)\right) \int_0^\infty L(R,r)\, p(r,t)\,\mathrm{d}r, \\ p(R,0) &= p_0(R), \end{aligned} \tag{3.1}$$

where the radial interaction kernel L is given by

$$L(R,r) = \frac{3}{16\pi\sigma^3} \frac{\min\{(R+r)^2,\sigma^2\} - \min\{(R-r)^2,\sigma^2\}}{R\,r}. \tag{3.2}$$

Proof. Let $K : [0,\infty) \to [0,\infty)$ be defined by $K(|x|) = k(x)$ and $L : [0,\infty) \to \mathbb{R}$ be defined by

$$L'(r^2) = K(r), \tag{3.3}$$

which can be computed explicitly

$$L(r) = \frac{3}{4\pi\sigma^3}\min\{r,\sigma^2\}. \tag{3.4}$$

Since the initial condition is a radially symmetric function and equation (1.1) does not involve space derivatives, the solution is a radially symmetric function. Let $p(R,t) = 4\pi R^2 n((0,0,R),t)$, where $R = |x| = (x_1^2 + x_2^2 + x_3^2)^{1/2}$. We fix such $x \in \mathbb{R}^3$ and $R \geq 0$. One can make two simple observations. First, points (x_1, x_2, x_3) and $(0,0,R)$ are in the same distance from zero. Second, the convolution $k * n$ is also a radially symmetrical function. Therefore we have

$$\begin{aligned} k * n(x,t) &= k * n((0,0,R),t) \\ &= \int_{\mathbb{R}^3} K\left(\left((0-y_1)^2 + (0-y_2)^2 + (R-y_3)^2\right)^{1/2}\right) n((y_1,y_2,y_3),t)\,\mathrm{d}y \\ &= \int_{\mathbb{R}^3} K\left(\left(y_1^2 + y_2^2 + y_3^2 + R^2 - 2R\,y_3\right)^{1/2}\right) \frac{p\left(\left(y_1^2+y_2^2+y_3^2\right)^{1/2}, t\right)}{4\pi\left(\left(y_1^2+y_2^2+y_3^2\right)^{1/2}\right)^2}\,\mathrm{d}y. \end{aligned} \tag{3.5}$$

To transform (1.1) to polar coordinates, we substitute

$$y_1 = r\cos\alpha\cos\beta, \quad y_2 = r\sin\alpha\cos\beta, \quad y_3 = r\sin\beta, \tag{3.6}$$

where $r > 0$, $0 \leq \alpha \leq 2\pi$ and $-\frac{\pi}{2} \leq \beta \leq \frac{\pi}{2}$. The Jacobian determinant of the change of variables in (3.6) is equal to $r^2\cos\beta$. Applying

$$r^2 = y_1^2 + y_2^2 + y_3^2, \qquad 2R\,y_3 = 2R\,r\sin\beta$$

to (3.5), we get the following

$$\begin{aligned} &\int_0^\infty \int_0^{2\pi} \int_{-\pi/2}^{\pi/2} K\left((r^2 + R^2 - 2R\,r\sin\beta)^{1/2}\right) \frac{p(r,t)}{4\pi r^2}\, r^2 \cos\beta\,\mathrm{d}\beta\,\mathrm{d}\alpha\,\mathrm{d}r \\ &\quad = \frac{1}{2}\int_0^\infty \int_{-\pi/2}^{\pi/2} K\left((r^2 + R^2 - 2R\,r\sin\beta)^{1/2}\right) p(r,t)\cos\beta\,\mathrm{d}\beta\,\mathrm{d}r \\ &\quad = \frac{1}{4R}\int_0^\infty \int_{(R-r)^2}^{(R+r)^2} K(u^{1/2})\,p(r,t)\,\frac{1}{r}\,\mathrm{d}u\,\mathrm{d}r, \end{aligned}$$

where the last equality comes from the substitution $u = r^2 + R^2 - 2\,R\,r\sin\beta$. Now, integrating with respect to u and using function L from (3.3), we obtain

$$K * p(R,t) = \frac{1}{4}\int_0^\infty \frac{L((R+r)^2) - L((R-r)^2)}{R\,r}\,p(r,t)\,\mathrm{d}r.$$

Using (3.4), we deduce

$$K * p(R,t) = \frac{3}{16\pi\,\sigma^3}\int_0^\infty \frac{\min\{(R+r)^2,\sigma^2\} - \min\{(R-r)^2,\sigma^2\}}{R\,r}\,p(r,t)\,\mathrm{d}r.$$

All together we obtain (3.1). □

In what follows it will be useful to introduce

$$\widetilde{L}(R,r) := \min\{(R+r)^2,\sigma^2\} - \min\{(R-r)^2,\sigma^2\}, \qquad \mathcal{C}_\sigma := \frac{3}{16\pi\,\sigma^3}, \tag{3.7}$$

so that $L(R,r) = \mathcal{C}_\sigma\,\frac{\widetilde{L}(R,r)}{R\,r}$. We conclude with a lemma collecting useful properties of $\widetilde{L}(R,r)$ and $L(R,r)$.

LEMMA 3.2 Let $L(R,r)$ and $\widetilde{L}(R,r)$ be given with (3.2) and (3.7), respectively. Then,

(P1) $0 \le L(R,r) \le 4\,\mathcal{C}_\sigma$,

(P2) $\widetilde{L}(R,r) \le 2\sigma^2$, $|\partial_R \widetilde{L}(R,r)| \le 4\sigma$ and $\widetilde{L}(R,r) \in BL(\mathbb{R}^+)$ with norm $4\sigma^2 + 4\sigma$,

(P3) $\left|\partial_R L(R,r)\right| \le \frac{1}{R}\left(\frac{2\sigma\,\mathcal{C}_\sigma}{r} + L(R,r)\right)$,

(P4) $L(R,r)$ is supported only on the set $|R-r| \le \sigma$,

(P5) $\frac{\widetilde{L}(R,r)}{R} \le 8\,\sigma$,

(P6) $r^2\,L(R,r) \le 16\,\sigma^2\,\mathcal{C}_\sigma$,

(P7) $\left|\int_{\mathbb{R}^+} L(R,r)\,\psi(R)\,\mathrm{d}R\right| \le 8\,\sigma\,\mathcal{C}_\sigma\,\|\psi\|_\infty$ for all bounded ψ,

(P8) $\left|\int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{R}\,\psi(R)\,\mathrm{d}R\right| \le 16\,\sigma^2\|\psi\|_\infty$ for all bounded ψ,

(P9) $r \mapsto \int_{\mathbb{R}^+} \psi(R)\,\widetilde{L}(R,r)\,\mathrm{d}R \in BL(\mathbb{R}^+)$ with norm $4\,\sigma^3\|\psi\|_\infty + 8\,\sigma^2\|\psi\|_\infty$.

Proof. First, we prove (P1), (P2) and (P3) simultaneously distinguishing four cases.

(1) If $|R+r| \le \sigma$ and $|R-r| \le \sigma$ we have $L(R,r) = 4\,\mathcal{C}_\sigma$ and $\widetilde{L}(R,r) = 4Rr$, so that (P1) is satisfied. For (P2) we have $\widetilde{L}(R,r) \le 2\sigma^2$, $\partial_R \widetilde{L}(R,r) = 4r \le 4\sigma$ and $\partial_r \widetilde{L}(R,r) = 4R \le 4\sigma$, because $0 \le r, R \le \sigma$. Finally, (P3) is clear because $\partial_R L(R,r) = 0$.

(2) If $|R+r| \ge \sigma$ and $|R-r| \ge \sigma$ we have $L(R,r) = 0$ and the conclusion is obvious.

(3) If $|R+r| \ge \sigma$ and $|R-r| \le \sigma$ we have $L(R,r) = \mathcal{C}_\sigma\,\frac{\sigma^2-(R-r)^2}{Rr}$. As $\sigma^2 \le (R+r)^2$, we have

$$L(R,r) = \mathcal{C}_\sigma\,\frac{\sigma^2 - (R-r)^2}{Rr} \le \mathcal{C}_\sigma\,\frac{(R+r)^2 - (R-r)^2}{Rr} = 4\,\mathcal{C}_\sigma$$

so (P1) is proved. To prove (P2) we note that $\widetilde{L}(R,r) = \sigma^2 - (R-r)^2 \le \sigma^2$. Then,

$$\partial_R \widetilde{L}(R,r) = -\partial_r \widetilde{L}(R,r) = -(R-r),$$

which is bounded by σ. For (P3) we observe that

$$\partial_R L(R,r) = \mathcal{C}_\sigma \, \frac{-(R-r)Rr - (\sigma^2 - (R-r)^2)\, r}{R^2 r^2} = -\mathcal{C}_\sigma \, \frac{R-r}{Rr} - \mathcal{C}_\sigma \, \frac{\sigma^2 - (R-r)^2}{R^2 r}.$$

For the first term we have $\mathcal{C}_\sigma \, \left|\frac{R-r}{Rr}\right| \leq \mathcal{C}_\sigma \, \frac{\sigma}{Rr}$ while the second is simply $-\frac{L(R,r)}{R}$.

(4) As $|R-r| \leq R + r = |R+r|$ there is no case $|R+r| < \sigma$ and $|R-r| > \sigma$.

Then, (P4) follows from the second case while (P5) is a consequence of (P1) and (P4). Indeed, when $r \leq 2\sigma$, we can estimate $\frac{\widetilde{L}(R,r)}{R} = \frac{1}{\mathcal{C}_\sigma}\, r\, L(R,r) \leq 4\,\sigma\, r \leq 8\sigma$. On the other hand, when $r \geq 2\sigma$, we can assume $R \geq \sigma$ so that $\frac{\widetilde{L}(R,r)}{R} \leq \frac{2\sigma^2}{\sigma} = 2\sigma$. To prove (P6) we proceed in the similar manner. If $r \leq 2\sigma$ we can estimate $r^2\, L(R,r) \leq 4\sigma^2\, 4\, \mathcal{C}_\sigma \leq 16\, \sigma^2\, \mathcal{C}_\sigma$. Otherwise, $R \geq r - \sigma$ so

$$r^2\, L(R,r) \leq \mathcal{C}_\sigma \, \frac{r}{r-\sigma}\, \widetilde{L}(R,r) = \frac{\mathcal{C}_\sigma}{1 - \sigma/r}\, \widetilde{L}(R,r) \leq \frac{\mathcal{C}_\sigma}{1 - 1/2}\, \widetilde{L}(R,r) \leq 4\, \sigma^2\, \mathcal{C}_\sigma.$$

To prove (P7) we use (P4) and (P1):

$$\left|\int_{\mathbb{R}^+} L(R,r)\, \psi(R)\, \mathrm{d}R\right| = \left|\int_{\mathbb{R}^+} L(R,r)\, \mathbb{1}_{|R-r|\leq\sigma}\, \psi(R)\, \mathrm{d}R\right| \leq 4\, \mathcal{C}_\sigma\, \|\psi\|_\infty \int_{\mathbb{R}^+} \mathbb{1}_{|R-r|\leq\sigma}\, \mathrm{d}R = 8\, \mathcal{C}_\sigma\, \sigma\, \|\psi\|_\infty,$$

as the measure of the set $|R-r| \leq \sigma$ equals 2σ. Assertion (P8) is proved similarly, using (P5) instead of (P1). Finally, to prove (P9), we first observe that the map of interest is bounded as due to (P2) and (P4), we have

$$\left|\int_{\mathbb{R}^+} \widetilde{L}(R,r)\, \psi(R)\, \mathrm{d}R\right| = \left|\int_{\mathbb{R}^+} \widetilde{L}(R,r)\, \mathbb{1}_{|R-r|\leq\sigma}\, \psi(R)\, \mathrm{d}R\right| \leq 2\sigma^2 \|\psi\|_\infty \int_{\mathbb{R}^+} \mathbb{1}_{|R-r|\leq\sigma}\, \mathrm{d}R = 4\sigma^3 \|\psi\|_\infty.$$

Similarly, using (P2), we prove that $\left|\int_{\mathbb{R}^+} \partial_r \widetilde{L}(R,r)\, \psi(R)\, \mathrm{d}R\right| \leq 8\sigma^2 \|\psi\|_\infty$ and this concludes the proof of (P9) thanks to Radamacher's Theorem, cf. Lemma 2.1 (D). □

4. Measure solutions to the radial equation

The solution to the numerical scheme is represented as a generalized solution being a measure rather than just a function. This section is devoted to the formulation of radial equation (1.2) in the space of measures.

We introduce

$$E_T = C(0,T; (\mathcal{M}_w^+(\mathbb{R}^+), \|\cdot\|_{BL^*,w})),$$

to be the space of continuous curves indexed with time $t \in [0,T]$ and valued in $(\mathcal{M}_w^+(\mathbb{R}^+), \|\cdot\|_{BL^*,w})$. Here, $\mathcal{M}_w^+(\mathbb{R}^+)$ is the subspace of non-negative measures vanishing linearly at $r = 0$, cf. (2.8), and

$\|\cdot\|_{BL^*,w}$ is defined with (2.9). Space E_T is equipped with the usual supremum norm

$$\|\mu_\bullet\|_{E_T} = \sup_{t\in[0,T]} \|\mu_t\|_{BL^*,w}. \tag{4.1}$$

We write λ for the Lebesgue measure on $\mathbb{R}^+$ and let $S(R) = 4\pi R^2$.

DEFINITION 4.1 (Mild measure solution). We say that $\mu_\bullet = \{\mu_t\}_{t\in[0,T]} \in E_T$ is a mild measure solution to (1.2) with initial condition $\mu_0 \in \mathcal{M}_w^+(\mathbb{R}^+)$ if for all test functions $\psi \in BL(\mathbb{R}^+)$, we have

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\mu_t(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, e^{-\int_0^t\int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_s(r)\,\mathrm{d}s}\,\mathrm{d}\mu_0(R)$$
$$+ \int_0^t \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, e^{-\int_s^t\int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u}\, L(R,r)\, S(R)\,\mathrm{d}\mu_s(r)\,\mathrm{d}\lambda(R)\,\mathrm{d}s. \tag{4.2}$$

NOTATION 4.2 It is convenient to define for $\mu_\bullet \in E_T$, $R \in \mathbb{R}^+$ and $s,t \in [0,T]$ with $s < t$

$$\mathcal{E}[\mu_\bullet, R, s, t] := e^{-\int_s^t\int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u}. \tag{4.3}$$

Motivation for Definition 4.1: Suppose that μ_t is a measure given by a continuous density $p(r,t)$ so that $\mu_t(A) = \int_A p(r,t)\,\mathrm{d}\mu_t(r)$. As (4.2) holds for all $\psi \in BL(\mathbb{R}^+)$, we discover

$$\frac{p(R,t)}{R} = e^{-\int_0^t\int_{\mathbb{R}^+} L(R,r)\,p(r,s)\,\mathrm{d}s}\,\frac{p(R,0)}{R} + \int_0^t\int_{\mathbb{R}^+} \frac{1}{R}\, e^{-\int_s^t\int_{\mathbb{R}^+} L(R,r)\,p(r,u)\,\mathrm{d}u}\, L(R,r)\,S(R)\,p(r,s)\,\mathrm{d}r\,\mathrm{d}s.$$

We multiply with $R > 0$ to get

$$p(R,t) = e^{-\int_0^t\int_{\mathbb{R}^+} L(R,r)\,p(r,s)\,\mathrm{d}s}\,p(R,0) + \int_0^t\int_{\mathbb{R}^+} e^{-\int_s^t\int_{\mathbb{R}^+} L(R,r)\,p(r,u)\,\mathrm{d}u}\, L(R,r)\,S(R)\,p(r,s)\,\mathrm{d}r\,\mathrm{d}s.$$

This is precisely variation-of-constants formula (or Duhamel formula) for (1.2). Thus, Definition 4.1 provides a generalization of the concept of classical solutions to (1.2). The factor $\frac{1}{R}$ is designed to study solutions that decay at least linearly when $R \to 0$.

The main result of this section reads:

THEOREM 4.3 Suppose that μ_0 is such that $\left\|\frac{\mu_0}{r^2}\right\|_{TV}, \left\|\frac{\mu_0}{r}\right\|_{TV}, \left\|\mu_0\right\|_{TV} < \infty$. Then, there exists a unique non-negative mild measure solution to (1.2) in E_T with initial condition μ_0. It satisfies the bound

$$\|\mu_t\|_{BL^*,w} \le \|\mu_0\|_{BL^*,w}\, e^{C(\sigma)t}, \qquad \|\mu_t\|_{TV} \le \|\mu_0\|_{TV}\, e^{C(\sigma)t}, \tag{4.4}$$

for some constant $C(\sigma)$ depending only on σ. Moreover, the solution is Lipschitz continuous in time

$$\|\mu_{t_2} - \mu_{t_1}\|_{BL^*,w} \le C_d\,|t_2 - t_1|. \tag{4.5}$$

Furthermore, if $\mu_t^{(1)}, \mu_t^{(2)}$ are measure solutions with initial conditions $\mu_0^{(1)}, \mu_0^{(2)}$ satisfying assumptions above, we have

$$\left\|\mu_t^{(1)} - \mu_t^{(2)}\right\|_{BL^*,w} \leq C_d \left\| \frac{\mu_0^{(1)} - \mu_0^{(2)}}{r\min(1,r)} \right\|_{BL^*}. \tag{4.6}$$

The constant C_d depends on data and $\left\|\frac{\mu_0}{r^2}\right\|_{TV}, \|\mu_0\|_{BL^*,w}, \left\|\frac{\nu_0}{r^2}\right\|_{TV}, \|\nu_0\|_{BL^*,w}$.

REMARK 4.4 Note that we have in mind the situation when μ_0 is a measure with density $p(r) = 4\pi r^2 n_0(0,0,r)$ where $n_0 \in L^\infty(\mathbb{R}^3)$ and has compact support, cf. Theorem 3.1, so that μ_0, $\frac{\mu_0}{r}$ and $\frac{\mu_0}{r^2}$ are bounded in the total variation norm.

The proof of Theorem 4.3 relies on continuity properties of (RHS) of (4.2). To this end, given $\mu_\bullet, \nu_\bullet \in E_T$, two measures $\gamma_1, \gamma_2 \in \mathcal{M}_w^+(\mathbb{R}^+)$ and $\psi \in BL(\mathbb{R}^+)$, we define two families of measures with

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\widetilde{\mu}_t(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}[\mu_\bullet, R, 0, t]\,\mathrm{d}\gamma_1(R) + \int_0^t \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}[\mu_\bullet, R, s, t]\,L(R,r)\,S(R)\,\mathrm{d}\mu_s(r)\,\mathrm{d}R\,\mathrm{d}s =: X_1 + Y_1, \tag{4.7}$$

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\widetilde{\nu}_t(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}[\nu_\bullet, R, 0, t]\,\mathrm{d}\gamma_2(R) + \int_0^t \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}[\nu_\bullet, R, s, t]\,L(R,r)\,S(R)\,\mathrm{d}\nu_s(r)\,\mathrm{d}R\,\mathrm{d}s =: X_2 + Y_2. \tag{4.8}$$

REMARK 4.5 We will prove in Lemma 4.8 that there exist unique families of measures $\{\widetilde{\mu}_t\}_{t\in[0,T]}$ and $\{\widetilde{\nu}_t\}_{t\in[0,T]}$ in $\mathcal{M}_w^+(\mathbb{R}^+)$ satisfying (4.7) and (4.8), respectively. In other words, formulas (4.7) and (4.8) define measures $\widetilde{\mu}_t$ and $\widetilde{\nu}_t$, respectively.

NOTATION 4.6 (Constant C_d). For the sake of simplicity we introduce constant C_d, which may differ from line to line and is allowed to depend continuously on data, i.e.

$$L,\ \sigma,\ T,\ \left\|\frac{\gamma_1}{r^2}\right\|_{TV},\ \left\|\frac{\gamma_2}{r^2}\right\|_{TV},\ \|\mu_\bullet\|_{E_T},\ \|\nu_\bullet\|_{E_T}.$$

LEMMA 4.7 (Continuity of $\mathcal{E}$). Under the notation above $\mathcal{E}$ enjoys the following properties:

(E1) boundedness: $0 \leq \mathcal{E}[\mu_\bullet, R, s, t] \leq 1$,

(E2) continuity with respect to measure argument:

$$|\mathcal{E}[\mu_\bullet, R, s, t] - \mathcal{E}[\nu_\bullet, R, s, t]| \leq \frac{C(\sigma)}{R}\int_s^t \|\mu_u - \nu_u\|_{BL^*,w}\,\mathrm{d}u,$$

(E3) continuity with respect to time: for all $v \leq s, t \leq T$, we have

$$\sup_{R \in \mathbb{R}^+} \left| \mathcal{E}[\mu_\bullet, R, v, t] - \mathcal{E}[\mu_\bullet, R, v, s] \right| \leq \frac{C_d}{R} \, |t-s|,$$

(E4) continuity with respect to R: the map $\mathbb{R} \ni R \mapsto \min(R,1)\, \mathcal{E}[\mu_\bullet, R, s, t]$ is in $BL(\mathbb{R}^+)$ with norm bounded by $C(\sigma, \|\mu_\bullet\|_{E_T})$.

Proof. Assertion (E1) is obvious. For (E2) we compute:

$$\begin{aligned}
\left| e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} - e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\nu_u(r)\,\mathrm{d}u} \right| &\leq \left| \int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}(\mu_u - \nu_u)(r)\,\mathrm{d}u \right| \\
&\leq \frac{\mathcal{C}_\sigma}{R} \left| \int_s^t \int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{r}\,\mathrm{d}(\mu_u - \nu_u)(r)\,\mathrm{d}u \right| \leq \mathcal{C}_\sigma \, \frac{4\sigma^2 + 4\sigma}{R} \int_0^t \|\mu_u - \nu_u\|_{BL^*,w}\,\mathrm{d}u,
\end{aligned}$$

where we used that the function e^x is 1-Lipschitz for $x \leq 0$ and that $\widetilde{L}(R,r)$ is jointly in $BL(\mathbb{R}^+)$ with constant $4\sigma^2 + 4\sigma$, cf. Lemma 3.2 (P2). To verify (E3) we compute similarly

$$\begin{aligned}
\left| e^{-\int_v^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} - e^{-\int_v^s \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} \right| &\leq \mathcal{C}_\sigma \int_s^t \int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{R\,r}\,\mathrm{d}\mu_u(r)\,\mathrm{d}u \\
&\leq \mathcal{C}_\sigma \, \frac{4\sigma^2 + 4\sigma}{R} \, \|\mu_\bullet\|_{E_T} \, |t-s|.
\end{aligned}$$

To demonstrate (E4) we first note that the map is bounded thanks to (E1). To prove Lipschitz continuity we use Radamacher's Theorem, cf. Lemma 2.1 (D). We observe that, owing to the product rule, the derivative of this map with respect to R equals

$$\mathbb{1}_{R \leq 1}\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} - \min(R,1)\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} \int_s^t \int_{\mathbb{R}^+} \partial_R L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u.$$

The first term is clearly bounded by 1 while for the second we estimate using Lemma 3.2 (P3):

$$\begin{aligned}
&\left| \min(R,1)\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} \int_s^t \int_{\mathbb{R}^+} \partial_R L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u \right| \\
&\qquad \leq \frac{\min(R,1)}{R}\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} \int_s^t \int_{\mathbb{R}^+} \frac{2\,\sigma\,\mathcal{C}_\sigma}{r}\,\mathrm{d}\mu_u(r)\,\mathrm{d}u \\
&\qquad\quad + \frac{\min(R,1)}{R}\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u} \int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u := X + Y.
\end{aligned}$$

Term X is bounded because $\frac{\min(R,1)}{R} \leq 1$ and $\int_{\mathbb{R}^+} \frac{2\,\sigma\,\mathcal{C}_\sigma}{r}\,\mathrm{d}\mu_s(r) \leq 2\,\sigma\,\mathcal{C}_\sigma \|\mu_\bullet\|_{E_T}$. Term Y is bounded because the function $x\,e^{-x}$ is bounded for $x \geq 0$. □

LEMMA 4.8 (*A priori* estimate). There exists a unique family of measures $\{\widetilde{\mu}_t\}_{t\in[0,T]} \subset \mathcal{M}_w^+(\mathbb{R}^+)$ such that (4.7) holds true. Moreover, there is a constant $C(\sigma)$ depending only on σ such that

$$\|\widetilde{\mu}_t\|_{BL^*,w} \leq \|\gamma_1\|_{BL^*,w} + C(\sigma)\int_0^t \|\mu_s\|_{BL^*,w}\,\mathrm{d}s. \tag{4.9}$$

Similarly,

$$\|\widetilde{\mu}_t\|_{TV} \leq \|\gamma_1\|_{TV} + C(\sigma)\int_0^t \|\mu_s\|_{TV}\,\mathrm{d}s. \tag{4.10}$$

Proof. We will use Riesz–Kakutani–Markov theorem (Rudin, 1987, Theorem 2.14), which asserts that any non-negative functional (not necessarily continuous!) on $C_c(\mathbb{R}^+)$ (i.e. space of continuous compactly supported functions on $\mathbb{R}^+$) defines a measure. We define functional with (RHS) of (4.7) as follows:

$$\begin{aligned}\mathcal{F}_t(\psi) = &\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}[\mu_\bullet, R, 0, t]\,\mathrm{d}\gamma_1(R)\\ &+\int_0^t\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\frac{\psi(R)}{R}\,\mathcal{E}[\mu_\bullet, R, s, t]\,L(R,r)\,S(R)\,\mathrm{d}\mu_s(r)\,\mathrm{d}R\,\mathrm{d}s.\end{aligned} \tag{4.11}$$

As $\mathcal{E}[\mu_\bullet, R, s, t] \in [0,1]$ the first term is bounded with $\|\psi\|_\infty \left\|\frac{\gamma_1}{R}\right\|_{TV} = \|\psi\|_\infty \|\gamma_1\|_{BL^*,w}$. In the second term we write $\frac{\psi(R)}{R}\,L(R,r)\,S(R) = 4\pi\,\mathcal{C}_\sigma\,\psi(R)\,\frac{\widetilde{L}(R,r)}{r}$. Thanks to Lemma 3.2 (P9) we have $\int_{\mathbb{R}^+}\psi(R)\,\mathcal{E}[\mu_\bullet, R, s, t]\,\widetilde{L}(R,r)\,\mathrm{d}R \leq \|\psi\|_\infty\,C(\sigma)$. Hence,

$$\begin{aligned}&\int_0^t\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\frac{\psi(R)}{R}\,\mathcal{E}[\mu_\bullet, R, s, t]\,L(R,r)\,S(R)\,\mathrm{d}\mu_s(r)\,\mathrm{d}R\,\mathrm{d}s\\ &\qquad\leq C(\sigma)\,\|\psi\|_\infty\int_0^t\int_{\mathbb{R}^+}\frac{1}{r}\,\mathrm{d}\mu_s(r)\,\mathrm{d}s = C(\sigma)\,\|\psi\|_\infty\int_0^t\|\mu_s\|_{BL^*,w}\,\mathrm{d}s.\end{aligned}$$

It follows that

$$\left|\mathcal{F}_t(\psi)\right| \leq \left(\|\gamma_1\|_{BL^*,w} + C(\sigma)\int_0^t\|\mu_s\|_{BL^*,w}\,\mathrm{d}s\right)\|\psi\|_\infty, \tag{4.12}$$

so that $\mathcal{F}_t$ is a functional on $C(\mathbb{R}^+)\cap L^\infty(\mathbb{R}^+)$, in particular, on $C_c(\mathbb{R}^+)$. Moreover, it is non-negative: if $\psi \geq 0$ then $\mathcal{F}(\psi) \geq 0$ by non-negativity of γ_1 and $\{\mu_t\}_{t\in[0,T]}$. It follows that there exists a family of measures $\{\widehat{\mu}_t\}_{t\in[0,T]}$ such that

$$\mathcal{F}_t(\psi) = \int_{\mathbb{R}^+}\psi(R)\,\mathrm{d}\widehat{\mu}_t(R). \tag{4.13}$$

Then, we define $\widetilde{\mu}_t(A) = \int_A R \, \mathrm{d}\widehat{\mu}_t(R)$ so that (4.11) and (4.13) implies

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathrm{d}\widetilde{\mu}_t(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathcal{E}[\mu_\bullet, R, 0, t] \, \mathrm{d}\gamma_1(R) \\ + \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathcal{E}[\mu_\bullet, R, s, t] \, L(R, r) \, S(R) \, \mathrm{d}\mu_s(r) \, \mathrm{d}R \, \mathrm{d}s, \tag{4.14}$$

which proves existence of $\{\widetilde{\mu}_t\}_{t\in[0,T]}$. Moreover, from (4.12), we deduce (4.9) so that $\left\|\widetilde{\mu}_t\right\|_{BL^*,w} < \infty$. To see uniqueness of $\left\{\widetilde{\mu}_t\right\}_{t\in[0,T]}$ we argue by contradiction. Suppose there are two families of measures $\left\{\widetilde{\mu}_t^{(1)}\right\}_{t\in[0,T]}, \left\{\widetilde{\mu}_t^{(2)}\right\}_{t\in[0,T]} \subset \mathcal{M}_w^+(\mathbb{R}^+)$ satisfying (4.14) so that for all $\psi \in BL(\mathbb{R}^+)$, we have

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathrm{d}\widetilde{\mu}_t^{(1)}(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathrm{d}\widetilde{\mu}_t^{(2)}(R).$$

Then, for all $t \in [0, T]$, we have $\widetilde{\mu}_t^{(1)}((a, b)) = \widetilde{\mu}_t^{(2)}((a, b))$ for all sub-intervals $(a, b) \subset (0, \infty)$. Hence, if $\widetilde{\mu}_t^{(1)} \neq \widetilde{\mu}_t^{(2)}$ for some $t \in [0, T]$, it has to be $\widetilde{\mu}_t^{(1)}\{0\} \neq \widetilde{\mu}_t^{(2)}\{0\}$. In particular, at least one of these measures, say $\widetilde{\mu}_t^{(1)}$, has an atom at 0, i.e. $\widetilde{\mu}_t^{(1)}\{0\} > 0$. But then,

$$\infty > \left\|\widetilde{\mu}_t^{(1)}\right\|_{BL^*,w} \geq \int_{\mathbb{R}^+} \frac{1}{R} \, \mathrm{d}\widetilde{\mu}_t^{(1)}(R) \geq \int_{\{0\}} \frac{1}{R} \, \mathrm{d}\widetilde{\mu}_t^{(1)}(R) = \infty,$$

raising contradiction. This concludes the proof of uniqueness. We proceed to the proof of the second estimate (4.10). We apply (4.11) with $\psi(R) := \psi_n(R)$ defined as

$$\psi_n(R) = \begin{cases} R & \text{if } 0 \leq R \leq n, \\ n\,(n + 1 - R) & \text{if } n \leq R \leq n + 1, \\ 0 & \text{if } R \geq n + 1. \end{cases}$$

Note that $\frac{\psi_n(R)}{R} \in [0, 1]$ and $\frac{\psi_n(R)}{R} \to 1$ monotonically as $n \to \infty$. As γ_1 is non-negative we easily deduce $\left|\int_{\mathbb{R}^+} \frac{\psi_n(R)}{R} \, \mathcal{E}[\mu_\bullet, R, 0, t] \, \mathrm{d}\gamma_1(R)\right| \leq \|\gamma_1\|_{TV} = \|\gamma_1\|_{BL^*}$. For the second term we first estimate

$$\left|\int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi_n(R)}{R} \, \mathcal{E}[\mu_\bullet, R, s, t] \, L(R, r) \, S(R) \, \mathrm{d}\mu_s(r) \, \mathrm{d}R \, \mathrm{d}s\right| \leq \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} L(R, r) \, S(R) \, \mathrm{d}\mu_s(r) \, \mathrm{d}R \, \mathrm{d}s.$$

Then, we split the integral for two cases: $R \geq 2\sigma$, $R \leq 2\sigma$ and denote the resulting integrals with I_1 and I_2, respectively. If $R \geq 2\sigma$ we use the support of L, cf. Lemma 3.2 (P4), to observe that $r \geq R - \sigma \geq \sigma$. Hence, $L(R, r) = \mathcal{C}_\sigma \, \frac{\widetilde{L}(R,r)}{R\,r} \leq \mathcal{C}_\sigma \, \frac{\widetilde{L}(R,r)}{R\,(R-\sigma)}$ and we have

$$L(R, r) \, S(R) = 4\pi \, \mathcal{C}_\sigma \, \widetilde{L}(R, r) \, \frac{R^2}{R\,(R - \sigma)} \leq 8\pi \, \mathcal{C}_\sigma \, \widetilde{L}(R, r) \text{ for } R \geq 2\sigma.$$

As $\int_{\mathbb{R}^+} \widetilde{L}(R,r)\,\mathrm{d}R \le C(\sigma)$ we deduce $I_1 \le C(\sigma)\int_0^t \|\mu_s\|_{TV}\,\mathrm{d}s$. The case $R \le \sigma$ corresponding to term I_2 is even easier because we can estimate $S(R) \le 4\pi\sigma^2$ and $\int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}R \le C(\sigma)$. It follows that

$$\int_{\mathbb{R}^+} \frac{\psi_n(R)}{R}\,\mathrm{d}\widetilde{\mu}_t(R) \le \|\gamma_1\|_{TV} + C(\sigma)\int_0^t \|\mu_s\|_{TV}\,\mathrm{d}s.$$

Application of monotone convergence theorem concludes the proof. □

LEMMA 4.9 (Continuity of Duhamel's formula wrt parameters). Let $\widetilde{\mu}_t$ and $\widetilde{\nu}_t$ be defined with (4.7) and (4.8), respectively. Then

$$\|\widetilde{\mu}_t - \widetilde{\nu}_t\|_{BL^*,w} \le C_d \left\| \frac{\gamma_1 - \gamma_2}{r\min(1,r)} \right\|_{BL^*} + C_d \int_0^t \|\mu_s - \nu_s\|_{BL^*,w}\,\mathrm{d}s. \tag{4.15}$$

Proof. Thanks to (4.7) and (4.8) we write for all $\psi \in BL(\mathbb{R}^+)$ with $\|\psi\|_{BL} \le 1$

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\widetilde{\mu}_t(R) = X_1 + Y_1, \qquad \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\widetilde{\nu}_t(R) = X_2 + Y_2,$$

where X_1 and Y_1 corresponds to the first and second summand in (4.7), respectively; similarly for X_2 and Y_2. To estimate $\|\widetilde{\mu}_t - \widetilde{\nu}_t\|_{BL^*,w}$ we write $\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\left(\widetilde{\mu}_t - \widetilde{\nu}_t\right)(R) = (X_1 - X_2) + (Y_1 - Y_2)$ and we estimate two differences separately.

<u>Term $X_1 - X_2$.</u> With triangle inequality this difference is controlled as

$$\left|\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}[\mu_\bullet, R, 0, t]\,\mathrm{d}\left(\gamma_1 - \gamma_2\right)(R)\right| + \left|\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\left(\mathcal{E}[\mu_\bullet, R, 0, t] - \mathcal{E}[\nu_\bullet, R, 0, t]\right)\mathrm{d}\gamma_2(R)\right|$$
$$=: Q_1 + Q_2.$$

For term Q_1, we write

$$Q_1 = \left|\int_{\mathbb{R}^+} \psi(R)\min(1,R)\,\mathcal{E}[\mu_\bullet, R, 0, t]\frac{\mathrm{d}\left(\gamma_1 - \gamma_2\right)(R)}{R\min(1,R)}\right|.$$

Note that $\|\psi\|_{BL} \le 1$ and $R \mapsto \min(1,R)\,\mathcal{E}[\mu_\bullet, R, 0, t] \in BL(\mathbb{R}^+)$ with norm controlled with C_d, cf. Lemma 4.7 (E4). Hence, the product of these functions also belongs to $BL(\mathbb{R}^+)$ with norm bounded by $2\,C_d$, cf. Lemma 2.1. It follows that

$$Q_1 \le C_d \left\| \frac{\gamma_1 - \gamma_2}{R\min(1,R)} \right\|_{BL^*}. \tag{4.16}$$

For term Q_2 we note that $\left|\mathcal{E}[\mu_\bullet, R, 0, t] - \mathcal{E}[\nu_\bullet, R, 0, t]\right| \le \frac{C_d}{R} \int_0^t \|\mu_s - \nu_s\|_{BL^*,w} \,\mathrm{d}s$ thanks to Lemma 4.7 (E2). Hence,

$$Q_2 \le C_d \int_0^t \|\mu_s - \nu_s\|_{BL^*,w} \,\mathrm{d}s \left\| \frac{\gamma_2}{R^2} \right\|_{TV} \le C_d \int_0^t \|\mu_s - \nu_s\|_{BL^*,w} \,\mathrm{d}s. \tag{4.17}$$

Term $Y_1 - Y_2$. To shorten formulas we introduce $\mathcal{E}^1(R, s) := \mathcal{E}[\mu_\bullet, R, s, t]$, $\mathcal{E}^2(R, s) := \mathcal{E}[\nu_\bullet, R, s, t]$. Aiming at triangle inequality again, we write

$$\begin{aligned} |Y_1 - Y_2| \le & \left| \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \left(\mathcal{E}^1(R, s) - \mathcal{E}^2(R, s)\right) L(R, r)\, S(R) \,\mathrm{d}\mu_s(r) \,\mathrm{d}R \,\mathrm{d}s \right| \\ & + \left| \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \mathcal{E}^2(R, s)\, L(R, r)\, S(R) \,\mathrm{d}(\mu_s - \nu_s)(r) \,\mathrm{d}R \,\mathrm{d}s \right| =: Z_1 + Z_2. \end{aligned}$$

For Z_1 we estimate $\left|\mathcal{E}^1(R, s) - \mathcal{E}^2(R, s)\right| \le \frac{C_d}{R} \int_s^t \|\mu_u - \nu_u\|_{BL^*,w} \,\mathrm{d}u$ using Lemma 4.7. Hence,

$$Z_1 \le C_d \int_0^t \|\mu_u - \nu_u\|_{BL^*,w} \,\mathrm{d}u \int_0^t \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \frac{|\psi(R)|}{R^2} L(R, r)\, S(R) \,\mathrm{d}R \right] \mathrm{d}\mu_s(r) \,\mathrm{d}s. \tag{4.18}$$

Now, we use $S(R) = 4\pi R^2$ and $L(R, r) = \mathcal{C}_\sigma \frac{\widetilde{L}(R,r)}{Rr}$, cf. (3.7). Thanks to Lemma 3.2 (P8) the integral $\int_{\mathbb{R}^+} \frac{|\psi(R)|}{R^2} \frac{\widetilde{L}(R,r)}{R} S_d(R) \,\mathrm{d}R$ is bounded with C_d. Hence,

$$\int_0^t \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \frac{|\psi(R)|}{R^2} L(R, r)\, S(R) \,\mathrm{d}R \right] \mathrm{d}\mu_s(r) \,\mathrm{d}s \le C_d \int_0^t \int_{\mathbb{R}^+} \frac{1}{r} \,\mathrm{d}\mu_s(r) \,\mathrm{d}s \le C_d\, t\, \|\mu_\bullet\|_{E_T},$$

cf. (4.1). From (4.18) we conclude that

$$Z_1 \le C_d \int_0^t \|\mu_s - \nu_s\|_{BL^*,w} \,\mathrm{d}s. \tag{4.19}$$

When it comes to term Z_2 we observe that $\frac{\psi(R)}{R} \mathcal{E}^2(R, s)\, L(R, r)\, S(R) = 4\pi\, \mathcal{C}_\sigma\, \psi(R)\, \mathcal{E}^2(R, s) \frac{\widetilde{L}(R,r)}{r}$. By Fubini Theorem

$$Z_2 = \int_0^t \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \frac{\psi(R)}{R} \mathcal{E}^2(R, s)\, L(R, r)\, S(R) \,\mathrm{d}R \right] \mathrm{d}(\mu_s - \nu_s)(r) \,\mathrm{d}s.$$

Hence, to bound the integrand in terms of $\|\mu_s - \nu_s\|_{BL^*,w}$, we only need to prove that the map $r \mapsto \int_{\mathbb{R}^+} \psi(R)\, \mathcal{E}^2(R, s)\, \widetilde{L}(R, r) \,\mathrm{d}R$ belongs to $BL(\mathbb{R}^+)$. As $\psi(R)\, \mathcal{E}^2(R, s)$ is bounded with $\|\psi\|_\infty$, this follows from Lemma 3.2 (P9). Hence,

$$Z_2 \le C_d \int_0^t \|\mu_s - \nu_s\|_{BL^*,w} \,\mathrm{d}s. \tag{4.20}$$

Collecting estimates (4.16), (4.17), (4.19) and (4.20) we conclude the proof of the lemma. □

LEMMA 4.10 (Continuity of Duhamel's formula wrt time). Let $\widetilde{\mu}_t$ be defined by (4.7). Then, under the notation above,

$$\left\| \widetilde{\mu_{t_1}} - \widetilde{\mu_{t_2}} \right\|_{BL^*,w} \leq C_d \, |t_1 - t_2|. \tag{4.21}$$

Proof. Thanks to (4.7), we have

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathrm{d}\widetilde{\mu_{t_1}}(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathcal{E}[\mu_\bullet, R, 0, t_1] \, \mathrm{d}\gamma_1(R)$$
$$+ \int_0^{t_1} \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathcal{E}[\mu_\bullet, R, u, t_1] \, L(R,r) \, S(R) \, \mathrm{d}\mu_u(r) \, \mathrm{d}R \, \mathrm{d}u =: G_1 + H_1,$$

and a similar expression for $\widetilde{\mu_{t_2}}$, which we split for $G_2 + H_2$. As in Lemma 4.9 we consider differences $G_1 - G_2$ and $H_1 - H_2$ separately. For term $G_1 - G_2$ we use $\left|\mathcal{E}[\mu_\bullet, R, 0, t_1] - \mathcal{E}[\mu_\bullet, R, 0, t_2]\right| \leq \frac{C_d}{R}|t_1 - t_2|$, cf. Lemma 4.7 (E3), to compute

$$|G_1 - G_2| \leq C_d \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \left|\mathcal{E}[\mu_\bullet, R, 0, t_1] - \mathcal{E}[\mu_\bullet, R, 0, t_2]\right| \, \mathrm{d}\gamma_1(R) \leq \|\psi\|_\infty \, C_d \, |t_1 - t_2| \, \left\| \frac{\gamma_1}{R^2} \right\|_{TV},$$

cf. Lemma 2.1 (A'). To estimate $H_1 - H_2$ we introduce auxiliary notation $\mathcal{E}^1(u,R) = \mathcal{E}[\mu_\bullet, R, u, t_1]$, $\mathcal{E}^2(u,R) = \mathcal{E}[\mu_\bullet, R, u, t_2]$ and get

$$|H_1 - H_2| \leq \int_{t_1}^{t_2} \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, \mathcal{E}^2(u,R) \, L(R,r) \, S(R) \, \mathrm{d}\mu_u(r) \, \mathrm{d}R \, \mathrm{d}u$$
$$+ \int_0^{t_1} \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \, (\mathcal{E}^2(u,R) - \mathcal{E}^1(u,R)) \, L(R,r) \, S(R) \, \mathrm{d}\mu_u(r) \, \mathrm{d}R \, \mathrm{d}u := K_1 + K_2.$$

To estimate K_1 we recall that $L(R,r) = \mathcal{C}_\sigma \, \frac{\widetilde{L}(R,r)}{Rr}$ and $S(R) = 4\pi R^2$ so that

$$K_1 \leq 4\pi \, \mathcal{C}_\sigma \, \int_{t_1}^{t_2} \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \psi(R) \, \mathcal{E}^2(u,R) \, \widetilde{L}(R,r) \, \mathrm{d}R \right] \frac{\mathrm{d}\mu_u(r)}{r} \, \mathrm{d}u$$
$$\leq C_d \int_{t_1}^{t_2} \int_{\mathbb{R}^+} \frac{\mathrm{d}\mu_u(r)}{r} \, \mathrm{d}u \leq C_d |t_1 - t_2| \|\mu_\bullet\|_{E_T} \leq C_d \, |t_1 - t_2|,$$

where we used Lemma 3.2 (P9) for the inner integral with respect to R. To estimate K_2 we use that $\left|\mathcal{E}^1(u,R) - \mathcal{E}^2(u,R)\right| \leq \frac{C_d}{R}|t_1 - t_2|$, cf. Lemma 4.7 (E3). Since $S(R) = 4\pi R^2$,

$$K_2 \leq 4\pi C_d \int_0^{t_1} \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \psi(R) \, |t_1 - t_2| \, L(R,r) \, \mathrm{d}\mu_u(r) \, \mathrm{d}R \, \mathrm{d}u$$
$$\leq C_d \, |t_1 - t_2| \int_0^{t_1} \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \psi(R) \, \frac{\widetilde{L}(R,r)}{R} \, \mathrm{d}R \right] \frac{\mathrm{d}\mu_u(r)}{r} \, \mathrm{d}u \leq C_d \, |t_1 - t_2| \, \|\mu_\bullet\|_{E_T} \leq C_d \, |t_1 - t_2|,$$

where we used Lemma 3.2 (P8) for the integral with respect to R. □

Now, we are in a position to prove Theorem 4.3.

Proof of Theorem 4.3. Let $P : E_T \to E_T$ be defined with (RHS) of (4.2), i.e. for $\mu_\bullet \in E_T$ we put

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, \mathrm{d}(P\mu_\bullet)_t(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, e^{-\int_0^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_s(r)\,\mathrm{d}s}\, \mathrm{d}\mu_0(R)$$
$$+ \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u(r)\,\mathrm{d}u}\, L(R,r)\, S(R)\, \mathrm{d}\mu_s(r)\, \mathrm{d}\lambda(R)\, \mathrm{d}s.$$

We define

$$K_T = \left\{ \nu_\bullet \in E_T : \nu_0 = \mu_0,\ \sup_{t\in[0,T]} \|\nu_t\|_{BL^*,w} \le 2\, \|\mu_0\|_{BL^*,w} \right\},$$

in order to find T_e such that $P : K_{T_e} \to K_{T_e}$ is contractive. Lemma 4.8 implies

$$\|(P\mu_\bullet)_t\|_{BL^*,w} \le \|\mu_0\|_{BL^*,w} + C(\sigma) \int_0^t \|\mu_s\|_{BL^*,w}\, \mathrm{d}s \le \|\mu_0\|_{BL^*,w} + C(\sigma)\, T_e\, 2\, \|\mu_0\|_{BL^*,w}.$$

Hence, $T_e \le 1/(2\, C(\sigma))$ and we only need to prove that P is contractive. Using Lemma 4.9 with $\gamma_1 = \gamma_2 := \mu_0$ we discover that there is some constant C_d depending on data such that

$$\|(P\mu_\bullet)_t - (P\nu_\bullet)_t\|_{BL^*,w} \le C_d \int_0^t \|\mu_s - \nu_s\|_{BL^*,w}\, \mathrm{d}s$$
$$\le C_d\, T_e \sup_{t\in[0,T_e]} \|\mu_\bullet - \nu_\bullet\|_{BL^*,w}.$$

Banach Fixed Point Theorem provides well-posedness for some small time depending on initial data $T_e = \min\left(\frac{1}{2C(\sigma)}, \frac{1}{2C_d}\right)$. But then Lemma 4.8 provides *a priori* estimate

$$\|\mu_t\|_{BL^*,w} \le \|\mu_0\|_{BL^*,w}\, e^{C(\sigma)\, t}, \qquad \|\mu_t\|_{TV} \le \|\mu_0\|_{TV}\, e^{C(\sigma)\, t}. \tag{4.22}$$

Hence, the solution does not blow up in finite time and we may repeat the argument presented above to cover arbitrarily large interval of time.

To prove continuity estimate, we first observe that in view of (4.22), μ_t is bounded by some constant depending on T, σ and the size of initial data with respect to $\|\cdot\|_{BL^*,w}$. Hence, constant C_d appearing in Lemmas 4.9 and 4.10 can be bounded in terms of

$$\left\|\frac{\mu_0}{r^2}\right\|_{BL^*},\ \left\|\frac{\nu_0}{r^2}\right\|_{BL^*},\ \|\mu_0\|_{BL^*,w},\ \|\nu_0\|_{BL^*,w},\ L,\ \sigma, T.$$

Applying Gronwall inequality to (4.15) we deduce (4.6), while (4.5) follows directly from (4.21). □

5. Solution to the numerical scheme as a measure solution

Now, we would like to find the connection between the numerical scheme (1.4) and measure solutions. The issue is that measure solutions to (1.2) are neither compactly supported nor concentrated at discrete points—a consequence of the infinite speed of propagation.

First, we deal with the support of solutions. The idea is to truncate the support and control the resulting error. The additional assumption made to handle these effects is that the initial datum has a certain decay at infinity. In particular, this is always satisfied for compactly supported initial datum.

ASSUMPTION 5.1 (Decay of initial condition μ_0). Let $M : \mathbb{R}^+ \to \mathbb{R}^+$ be a C^1 strictly increasing function with $\frac{M(r+\sigma)}{M(r)} \leq C_M(\sigma)$. We assume that $\mu_0 \in \mathcal{M}^+(\mathbb{R}^+)$ is such that $\int_{\mathbb{R}^+} \frac{M(r)}{r}\, \mathrm{d}\mu_0(r) < \infty$.

REMARK 5.2 We list here three examples of functions M satisfying condition $\frac{M(r+\sigma)}{M(r)} \leq C_M(\sigma)$.

(A) $M_1(r) = e^r$ with $\frac{M_1(r+\sigma)}{M_1(r)} = e^\sigma =: C_{M_1}(\sigma)$.

(B) $M_2(r) = (1+r)^k$ with $k \in \mathbb{N}$ and $\frac{M_2(r+\sigma)}{M_2(r)} \leq (1+\sigma)^k =: C_{M_2}(\sigma)$.

(C) If M is as in Assumption 5.1 then its truncation $M^k(r) := \begin{cases} M(r) & \text{if } r \leq k \\ M(k) & \text{if } r > k \end{cases}$ satisfies $\frac{M^k(r+\sigma)}{M^k(r)} \leq \max(1, C_M(\sigma))$. This is not trivial only if $r+\sigma > k$, while $r \leq k$. But then, by monotonicity of M,

$$\frac{M^k(r+\sigma)}{M^k(r)} = \frac{M(k)}{M(r)} \leq \frac{M(r+\sigma)}{M(r)} \leq C_M(\sigma).$$

THEOREM 5.3 (Truncation of support). Under Assumption 5.1 the mild measure solution to (1.2) with initial data μ_0 satisfies

$$\int_{\mathbb{R}^+} \frac{M(r)}{r}\, \mathrm{d}\mu_t(r) \leq \int_{\mathbb{R}^+} \frac{M(r)}{r}\, \mathrm{d}\mu_0(r)\, e^{Ct}, \qquad C = C(\sigma)\, \max(1, C_M(\sigma)). \tag{5.1}$$

In particular, we have an estimate on the tail of μ_t:

$$\left\| \mu_t|_{[0,R_0]} - \mu_t \right\|_{BL^*,w} \leq \frac{1}{M(R_0)} \left[\int_{\mathbb{R}^+} \frac{M(r)}{r}\, \mathrm{d}\mu_0(r) \right] e^{Ct},$$

where $\mu_t|_{[0,R_0]}$ is restriction of μ_t to the interval $[0, R_0]$.

Proof of Theorem 5.3. We want to use the definition of measure solution (4.2) with test function $\psi(R) = M(R)$, but this is not an admissible test function, so we fix $k \in \mathbb{N}$ and consider truncation M^k as in Remark 5.2 (C). Hence, we have

$$\int_{\mathbb{R}^+} \frac{M^k(R)}{R}\, \mathrm{d}\mu_t(R) = \int_{\mathbb{R}^+} \frac{M^k(R)}{R}\, \mathcal{E}[\mu_\bullet, R, 0, t]\, \mathrm{d}\mu_0(R)$$
$$+ \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{M^k(R)}{R}\, \mathcal{E}[\mu_\bullet, R, s, t]\, L(R, r)\, S(R)\, \mathrm{d}\mu_s(r)\, \mathrm{d}R\, \mathrm{d}s =: X + Y. \tag{5.2}$$

Term X is trivially controlled by $|X| \leq \int_{\mathbb{R}^+} \frac{M^k(R)}{R}\, \mathrm{d}\mu_0(R)$. For term Y we write $L(R,r) = \mathcal{C}_\sigma \frac{\widetilde{L}(R,r)}{R\,r}$ and note that $\frac{S(R)}{R^2} = 4\pi$ so that

$$
\begin{aligned}
|Y| &= \mathcal{C}_\sigma \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{M^k(R)}{R}\, \mathcal{E}[\mu_\bullet, R, s, t]\, \frac{\widetilde{L}(R,r)}{R\,r}\, S(R)\, \mathrm{d}\mu_s(r)\, \mathrm{d}R\, \mathrm{d}s \\
&= 4\pi\, \mathcal{C}_\sigma \int_0^t \int_{\mathbb{R}^+} \left(\int_{\mathbb{R}^+} \frac{M^k(R)}{M^k(r)}\, \widetilde{L}(R,r)\, \mathrm{d}R \right) \frac{M^k(r)}{r}\, \mathrm{d}\mu_s(r)\, \mathrm{d}s.
\end{aligned}
\tag{5.3}
$$

As $\widetilde{L}(R,r)$ is supported only on $|R-r| \leq \sigma$, we can use monotonicity (not necessarily strict monotonicity) of M^k and Assumption 5.1 to estimate

$$
\begin{aligned}
\int_{\mathbb{R}^+} \frac{M^k(R)}{M^k(r)}\, \widetilde{L}(R,r)\, \mathrm{d}R &\leq \int_{\mathbb{R}^+} \frac{M^k(r+\sigma)}{M^k(r)}\, \widetilde{L}(R,r)\, \mathrm{d}R \\
&\leq C_M(\sigma) \int_{\mathbb{R}^+} \widetilde{L}(R,r)\, \mathrm{d}R \leq \max(1, C_M(\sigma))\, C(\sigma),
\end{aligned}
\tag{5.4}
$$

thanks to Lemma 3.2 (P9). Therefore, (5.3) implies

$$
|Y| \leq \max(1, C_M(\sigma))\, C(\sigma) \int_0^t \int_{\mathbb{R}^+} \frac{M^k(r)}{r}\, \mathrm{d}\mu_s(r)\, \mathrm{d}s.
$$

Using Gronwall's inequality, we deduce

$$
\int_{\mathbb{R}^+} \frac{M^k(r)}{r}\, \mathrm{d}\mu_t(r) \leq \int_{\mathbb{R}^+} \frac{M^k(r)}{r}\, \mathrm{d}\mu_0(r)\, e^{C\,t}, \qquad C = C(\sigma)\, \max(1, C_M(\sigma)).
$$

Then, $\int_{\mathbb{R}^+} \frac{M^k(r)}{r}\, \mathrm{d}\mu_0(r) \leq \int_{\mathbb{R}^+} \frac{M(r)}{r}\, \mathrm{d}\mu_0(r)$ and $M_k(r) \to M(r)$ increasingly, so monotone convergence theorem yields (5.1). The estimate on tail follows from simple computation:

$$
\left\| \mu_t|_{[0,R_0]} - \mu_t \right\|_{BL^*,w} = \left\| \mu_t|_{(R_0,\infty)} \right\|_{BL^*,w} = \int_{[R_0,\infty)} \frac{1}{r}\, \mathrm{d}\mu_t(r) \leq \frac{1}{M(R_0)} \int_{\mathbb{R}^+} \frac{M(r)}{r}\, \mathrm{d}\mu_t(r),
$$

where we used again monotonicity of M. □

Now, having the support truncated at R_0, we consider an equation in the space of measures

$$
\partial_t \mu_t^N = (\lambda_N\, S(R) - \mu_t^N) \int_{\mathbb{R}^+} L(R,r)\, \mathrm{d}\mu_t^N(r),
\tag{5.5}
$$

where $\lambda_N = \sum_{i=1}^N \frac{R_0}{N}\,\delta_{x_i}$ approximates the Lebesgue measure λ on $[0,R_0]$, $x_i := \frac{i}{N}R_0$ and (5.5) is understood in the usual mild sense as in Definition 4.1, i.e. for all test functions $\psi \in BL(\mathbb{R}^+)$, we have

$$\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\mu_t^N(R) = \int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, e^{-\int_0^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_s^N(r)\,\mathrm{d}s}\,\mathrm{d}\mu_0(R)$$
$$+ \int_0^t \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\, e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u^N(r)\,\mathrm{d}u}\, L(R,r)\,S(R)\,\mathrm{d}\mu_s^N(r)\,\mathrm{d}\lambda_N(R)\,\mathrm{d}s. \tag{5.6}$$

It turns out that solutions to the numerical scheme (1.4) can be written as a measure solution to (5.5).

THEOREM 5.4 Let $\mu_0 \in \mathcal{M}_w^+(\mathbb{R}^+)$ be as in Theorem 4.3 and suppose it satisfies Assumption 5.1. Let C_d be any constant depending on the size of the initial datum and model parameters. Let

$$\mu_0^N := \sum_{i=1}^N m_i^N(0)\,\delta_{x_i},$$

where $m_i^N(0) \in \mathbb{R}^+$ are given. Consider (5.5) with initial condition μ_0^N and $1 \le R_0 \le N$. Then, the unique non-negative measure solution is of the form $\mu_t^N = \sum_{i=1}^N m_i^N(t)\,\delta_{x_i}$, where $m_i^N(t)$ solve the numerical scheme (1.4). Moreover,

(A) we have estimates

$$\sup_{t\in[0,T]} \|\mu_t^N\|_{BL^*,w} \le \|\mu_0^N\|_{BL^*,w}\, e^{C(\sigma)\,T} \le C_d, \qquad \sup_{t\in[0,T]} \|\mu_t^N\|_{TV} \le \|\mu_0^N\|_{TV}\, e^{C(\sigma)\,T} \le C_d,$$

(B) discretization μ_t^N satisfies the same decay estimate as μ_t

$$\int_{\mathbb{R}^+} \frac{M(r)}{r}\,\mathrm{d}\mu_t^N(r) \le \int_{\mathbb{R}^+} \frac{M(r)}{r}\,\mathrm{d}\mu_0^N(r)\, e^{C\,t}, \qquad C = C(\sigma)\,\max(1, C_M(\sigma)),$$

(C) if $\widetilde{\mu}_t$ is a measure solution to (1.2) with initial data μ_0^N, we have

$$\left\|\widetilde{\mu}_t - \mu_t^N\right\|_{BL^*,w} \le \frac{C_d\,R_0^2}{N} + \frac{C_d}{M(R_0)}.$$

Proof. To prove the representation formula for μ_t^N we first take any ψ, which is not supported at knots $\{x_i\}_{1\le i\le N}$. From the definition of mild solution (5.6) we obtain that $\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\mu_t^N(R) = 0$, which implies that any non-negative mild measure solution is supported on the knots. Hence, we only need to find $m_i^N(t)$. To do that we take any ψ, which is supported only at one of the knots, say x_i. Because

$x_i \neq 0$, we have

$$m_i^N(t) = m_i^N(0)\, e^{-\int_0^t \int_{\mathbb{R}^+} L(x_i,r)\,\mathrm{d}\mu_s^N(r)\,\mathrm{d}s} + \int_0^t \int_{\mathbb{R}^+} e^{-\int_s^t \int_{\mathbb{R}^+} L(x_i,r)\,\mathrm{d}\mu_u^N(r)\,\mathrm{d}u}\, \frac{R_0}{N}\, S(x_i)\, L(x_i,r)\,\mathrm{d}\mu_s^N(r)\,\mathrm{d}s.$$

Using the support of μ_t^N we can write it as

$$m_i^N(t) = m_i^N(0)\, e^{-\int_0^t \sum_{j=1}^N L(x_i,x_j)\, m_j^N(s)\,\mathrm{d}s} + \int_0^t e^{-\int_s^t \sum_{j=1}^N L(x_i,x_j)\, m_j^N(u)\,\mathrm{d}u}\, \frac{R_0}{N}\, S(x_i) \sum_{j=1}^N L(x_i,x_j)\, m_j^N(s)\,\mathrm{d}s.$$

This is precisely the variation-of-constants formula for ODE (1.4).

For the proof of (A) we sum up equations (1.4) for $i = 1, ..., N$ to obtain

$$\partial_t \sum_{i=1}^N \frac{m_i^N(t)}{x_i} \leq \frac{R_0}{N} \sum_{i=1}^N \frac{4\pi x_i^2}{x_i} \sum_{j=1}^N L(x_i,x_j)\, m_j^N(t) = 4\pi\, \mathcal{C}_\sigma\, \frac{R_0}{N} \sum_{j=1}^N \sum_{i=1}^N 2\sigma^2 \mathbb{1}_{|x_i-x_j|\leq\sigma}\, \frac{m_j^N(t)}{x_j},$$

where we used that $L(x_i,x_j) = \mathcal{C}_\sigma \frac{\widetilde{L}(x_i,x_j)}{x_i x_j}$ is supported for $|x_i - x_j| \leq \sigma$ and that $\widetilde{L}(x_i,x_j) \leq 2\sigma^2$, cf. Lemma 3.2 (P2), (P4). Fix $j \in \{1, ..., N\}$ and observe that condition $|x_i - x_j| \leq \sigma$ is equivalent to $|i-j| \leq \frac{N}{R_0}\sigma$. There are at most $2\frac{N}{R_0}\sigma + 1 \leq \frac{N}{R_0}(2\sigma+1)$ points i satisfying this condition. It follows that $\sum_{i=1}^N \mathbb{1}_{|x_i-x_j|\leq\sigma} \leq \frac{N}{R_0}(2\sigma+1)$ and this implies

$$\partial_t \sum_{i=1}^N \frac{m_i^N(t)}{x_i} \leq 8\pi\sigma^2\, \mathcal{C}_\sigma\, \frac{R_0}{N}\, \frac{N}{R_0}\, (2\sigma+1) \sum_{j=1}^N \frac{m_j^N(t)}{x_j} \leq C(\sigma) \sum_{j=1}^N \frac{m_j^N(t)}{x_j}.$$

Applying Gronwall's inequality concludes the proof of the first estimate. To see the second one we proceed in a similar way, this time estimating

$$\partial_t \sum_{i=1}^N m_i^N(t) \leq \frac{R_0}{N} \sum_{i=1}^N 4\pi x_i^2 \sum_{j=1}^N L(x_i,x_j)\, m_j^N(t) = 4\pi\, \frac{R_0}{N} \sum_{j=1}^N \sum_{i=1}^N 2\sigma^2 \mathbb{1}_{|x_i-x_j|\leq\sigma}\, m_j^N(t),$$

where we used $r^2 L(R,r) \leq C(\sigma)$, cf. Lemma 3.2 (P6). We conclude in the same manner.

To prove (B) we can repeat the proof of Theorem 5.3. Indeed, the only problem one faces is to prove that $\int_{\mathbb{R}^+} \widetilde{L}(R,r)\,\mathrm{d}\lambda_N(R) \leq C(\sigma)$, where $\lambda_N = \frac{R_0}{N}\sum_{i=1}^N \delta_{x_i}$, cf. (5.4). However, we know that $\widetilde{L}(R,r)$ is supported for $|R-r| \leq \sigma$ and it is bounded with $C(\sigma)$, cf. Lemma 3.2 (P2), (P4). For fixed r there are at most $2\sigma/\left(\frac{N}{R_0}\right) + 1 \leq (2\sigma+1)\,\frac{R_0}{N}$ points x_i such that $|x_i - r| \leq \sigma$. Therefore,

$$\int_{\mathbb{R}^+} \widetilde{L}(R,r)\,\mathrm{d}\lambda_N(R) = \frac{R_0}{N} \sum_{i:|x_i-r|\leq\sigma} \widetilde{L}(r,x_i) \leq C(\sigma)\,\frac{R_0}{N}\,(2\sigma+1)\,\frac{R_0}{N} \leq C(\sigma).$$

To prove (C) we need to estimate $\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}(\widetilde{\mu}_t - \mu_t^N)$ uniformly in $\psi \in BL(\mathbb{R}^+)$ with $\|\psi\|_{BL} \leq 1$. We let $\mathcal{E}(s,t) = e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\widetilde{\mu_u}(r)\,\mathrm{d}u}$ and $\mathcal{E}^N(s,t) = e^{-\int_s^t \int_{\mathbb{R}^+} L(R,r)\,\mathrm{d}\mu_u^N(r)\,\mathrm{d}u}$. We have

$$\begin{aligned}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\widetilde{\mu}_t(R) = &\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}(0,t)\,\mathrm{d}\mu_0^N(R)\\ &+ \int_0^t \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}(s,t)\,L(R,r)\,S(R)\,\mathrm{d}\widetilde{\mu}_s(r)\,\mathrm{d}\lambda(R)\,\mathrm{d}s =: X_1 + Y_1,\end{aligned} \tag{5.7}$$

$$\begin{aligned}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathrm{d}\mu_t^N(R) = &\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}^N(0,t)\,\mathrm{d}\mu_0^N(R)\\ &+ \int_0^t \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \frac{\psi(R)}{R}\,\mathcal{E}^N(s,t)\,L(R,r)\,S(R)\,\mathrm{d}\mu_s^N(r)\,\mathrm{d}\lambda^N(R)\,\mathrm{d}s =: X_2 + Y_2.\end{aligned} \tag{5.8}$$

We subtract these identities and study two terms independently. Before proceeding to computations, we note an auxiliary estimate that follows from (E2) in Lemma 4.7:

$$\left|\mathcal{E}(s,t) - \mathcal{E}^N(s,t)\right| \leq \frac{C(\sigma)}{R}\int_s^t \left\|\widetilde{\mu_u} - \mu_u^N\right\|_{BL^*,w}\mathrm{d}u. \tag{5.9}$$

Term with initial conditions $|X_1 - X_2|$. We have $\|\psi\|_\infty \leq 1$ and $\|\mu_0^N\|_{TV} = \|\mu_0\|_{TV} \leq C_d$. Using (5.9), we obtain

$$|X_1 - X_2| \leq C(\sigma)\int_0^t \left\|\widetilde{\mu}_s - \mu_s^N\right\|_{BL^*,w}\mathrm{d}s\,\left\|\frac{\mu_0^N}{R^2}\right\|_{TV}. \tag{5.10}$$

We note that $\left\|\frac{\mu_0^N}{R^2}\right\|_{TV} = \left\|\frac{\mu_0}{R^2}\right\|_{TV}$ because with $A_1 = [0,x_1)$, $A_i = [x_{i-1},x_i)$ $(i = 2,...,n-1)$ and $A_n = [x_{n-1},x_n]$, we have

$$\left\|\frac{\mu_0^N}{R^2}\right\|_{TV} = \sum_{i=1}^N \frac{\mu_0(A_i)}{x_i^2} \leq \int_{[0,R_0]} \frac{1}{R^2}\,\mathrm{d}\mu_0(R) \leq \left\|\frac{\mu_0}{R^2}\right\|_{TV}.$$

Therefore, estimate (5.10) simplifies to

$$|X_1 - X_2| \leq C_d \int_0^t \left\|\widetilde{\mu}_s - \mu_s^N\right\|_{BL^*,w}\mathrm{d}s. \tag{5.11}$$

Term with nonlocal interactions $|Y_1 - Y_2|$. Aiming at triangle inequality, we write

$$
\begin{aligned}
|Y_1 - Y_2| \leq & \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \left(\mathcal{E}(s,t) - \mathcal{E}^N(s,t)\right) L(R,r)\, S(R)\, \mathrm{d}\widetilde{\mu}_s(r)\, \mathrm{d}\lambda(R)\, \mathrm{d}s \\
& + \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \mathcal{E}^N(s,t)\, L(R,r)\, S(R)\, \mathrm{d}\widetilde{\mu}_s(r)\, \mathrm{d}(\lambda - \lambda_N)(R)\, \mathrm{d}s \\
& + \int_0^t \int_{\mathbb{R}^+} \int_{\mathbb{R}^+} \frac{\psi(R)}{R} \mathcal{E}^N(s,t)\, L(R,r)\, S(R)\, \mathrm{d}(\widetilde{\mu}_s - \mu_s^N)(r)\, \mathrm{d}\lambda_N(R)\, \mathrm{d}s =: Z_1 + Z_2 + Z_3.
\end{aligned}
$$

Term Z_1. Note that $\|\psi\|_\infty \leq 1$ and $\|\widetilde{\mu}_s\|_{BL^*,w} \leq C_d$ due to the estimate (4.4). As $S(R) = 4\pi R^2$ we use (5.9) to obtain

$$
\begin{aligned}
Z_1 & \leq 4\pi\, \mathcal{C}_\sigma \int_0^t \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{R}\, \mathrm{d}\lambda(R) \right] \frac{\widetilde{\mathrm{d}\mu_s(r)}}{r}\, \mathrm{d}s \int_0^t \left\| \widetilde{\mu}_s - \mu_s^N \right\|_{BL^*,w} \mathrm{d}s \\
& \leq C_d \sup_{s\in[0,t]} \|\mu_s\|_{BL^*,w} \int_0^t \left\| \widetilde{\mu}_s - \mu_s^N \right\|_{BL^*,w} \mathrm{d}s \leq C_d \int_0^t \left\| \widetilde{\mu}_s - \mu_s^N \right\|_{BL^*,w} \mathrm{d}s, \qquad (5.12)
\end{aligned}
$$

where in the second estimate we used Lemma 3.2 (P8) to bound the integral $\int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{R}\, \mathrm{d}\lambda(R)$.

Term Z_2. First, we write

$$
Z_2 = 4\pi\, \mathcal{C}_\sigma \int_0^t \int_{\mathbb{R}^+} \psi(R)\, \mathcal{E}^N(s,t) \left[\int_{\mathbb{R}^+} \widetilde{L}(R,r)\, \frac{\mathrm{d}\widetilde{\mu}_s(r)}{r} \right] \mathrm{d}(\lambda - \lambda_N)(R)\, \mathrm{d}s,
$$

and then, we split the integral with respect to R for two subsets $R \in [0, R_0]$ and $R > R_0$, denoting the resulting integrals with $Z_2^{(1)}$ and $Z_2^{(2)}$. For $Z_2^{(1)}$ we consider the map

$$
R \mapsto \mathcal{G}(R) := \psi(R)\, \mathcal{E}^N(s,t) \left[\int_{\mathbb{R}^+} \widetilde{L}(R,r)\, \frac{\mathrm{d}\widetilde{\mu}_s(r)}{r} \right], \qquad (5.13)
$$

and Lemma 5.5 below shows that it belongs to $BL\left[0, R_0\right]$ with constant C_d. Thanks to Remark 2.4 concerning discretization of Lebesgue measure, we obtain

$$
Z_2^{(1)} \leq C_d \left\| \lambda - \lambda_N \right\|_{BL^*[0,R_0]} \leq C_d\, \frac{R_0^2}{N}. \qquad (5.14)
$$

To estimate $Z_2^{(2)}$ we observe that $L(R,r)$ is supported only for $|R - r| \leq \sigma$, cf. Lemma 3.2 4, so that we may restrict the integral with respect to r to the case $r \geq R_0 - \sigma$. Hence,

$$
Z_2^{(2)} = 4\pi\, \mathcal{C}_\sigma \int_0^t \int_{r \geq R_0 - \sigma} \left[\int_{R \geq R_0} \psi(R)\, \mathcal{E}^N(s,t)\, \widetilde{L}(R,r)\, \mathrm{d}\lambda(R) \right] \frac{\mathrm{d}\widetilde{\mu}_s(r)}{r}\, \mathrm{d}s.
$$

The inner integral is controlled with $C(\sigma)$ due to the Lemma 3.2 (P9). For the outer one we use the estimate on the tail from Theorem 5.3, namely

$$Z_2^{(2)} \leq \frac{C_d}{M(R_0-\sigma)} \int_0^t \int_{r\geq R_0-\sigma} M(r)\,\mathrm{d}\widetilde{\mu}_s(r)\,\mathrm{d}s \leq \frac{C_d\,C_M(\sigma)}{M(R_0)} \int_0^t C_M[\mu_s]\,\mathrm{d}s \leq \frac{C_d}{M(R_0)}, \tag{5.15}$$

where we used that $\frac{M(R_0)}{M(R_0-\sigma)} \leq C_M(\sigma)$.

Term Z_3. First, we write $\frac{1}{R}L(R,r)S(R) = 4\pi\,\mathcal{C}_\sigma\,\frac{\widetilde{L}(R,r)}{r}$. Hence,

$$Z_3 = 4\pi\,\mathcal{C}_\sigma \int_0^t \int_{\mathbb{R}^+} \left[\int_{\mathbb{R}^+} \psi(R)\,\mathcal{E}^N(s,t)\,\widetilde{L}(R,r)\,\mathrm{d}\lambda_N(R)\right] \frac{\mathrm{d}(\widetilde{\mu}_s-\mu_s^N)(r)}{r}\,\mathrm{d}s.$$

We observe that the function

$$r \mapsto \mathcal{F}(r) := \int_{\mathbb{R}^+} \psi(R)\,\mathcal{E}^N(s,t)\,\widetilde{L}(R,r)\,\mathrm{d}\lambda_N(R) \tag{5.16}$$

is in $BL(\mathbb{R}^+)$ with constant $C(\sigma)$ by Lemma 5.6 below. It follows that

$$Z_3 \leq C(\sigma) \int_0^t \left\|\widetilde{\mu}_s - \mu_s^N\right\|_{BL^*,w} \mathrm{d}s. \tag{5.17}$$

Conclusion. Collecting estimates (5.11), (5.12), (5.14), (5.15) and (5.17), we obtain

$$\left\|\widetilde{\mu}_t - \mu_t^N\right\|_{BL^*,w} \leq C_d \int_0^t \left\|\widetilde{\mu}_s - \mu_s^N\right\|_{BL^*,w} \mathrm{d}s + \frac{C_d\,R_0^2}{N} + \frac{C_d}{M(R_0)}.$$

Application of Gronwall concludes the proof (C). □

LEMMA 5.5 Let $\|\psi\|_{BL} \leq 1$. Under the notation of the proof of Theorem 5.4 the function defined in (5.13) belongs to $BL\left[0,R_0\right]$ with constant C_d.

Proof. First, the function $\mathcal{G}$ is bounded with

$$|\mathcal{G}(R)| \leq \|\psi\|_\infty \left|\mathcal{E}^N(s,t)\right| \|\widetilde{L}\|_\infty \sup_{s\in[0,t]} \|\widetilde{\mu}_s\|_{BL^*,w} \leq C(\sigma)\,C_d \leq C_d, \tag{5.18}$$

where we used $\|\psi\|_\infty \leq 1$, Lemma 4.7 (E1), Lemma 3.2 (P2) and estimate (4.4). Aiming at application of the Radamacher's Theorem, cf. Lemma 2.1 (D), we compute its derivative and we want to prove that it is uniformly bounded. We have

$$\begin{aligned}\partial_R\mathcal{G}(R) = {}& \partial_R\psi(R)\,\mathcal{E}^N(s,t)\left[\int_{\mathbb{R}^+} \widetilde{L}(R,r)\,\frac{\mathrm{d}\widetilde{\mu}_s(r)}{r}\right] + \psi(R)\,\partial_R\mathcal{E}^N(s,t)\left[\int_{\mathbb{R}^+} \widetilde{L}(R,r)\,\frac{\mathrm{d}\widetilde{\mu}_s(r)}{r}\right] \\ & + \psi(R)\,\mathcal{E}^N(s,t)\left[\int_{\mathbb{R}^+} \partial_R\widetilde{L}(R,r)\,\frac{\mathrm{d}\widetilde{\mu}_s(r)}{r}\right] =: (A) + (B) + (C).\end{aligned}$$

Term (A) is bounded by virtue of (5.18) because $\|\psi\|_{BL} \le 1$ implies $\|\partial_R \psi\|_\infty \le 1$. For the term (C) we observe that Lemma 3.2 (P2) implies that $\left|\partial_R \widetilde{L}(R,r)\right| \le C(\sigma)$ so that

$$|(C)| \le C(\sigma) \sup_{s\in[0,t]} \left\|\widetilde{\mu}_s\right\|_{BL^*,w} \le C_d.$$

The most difficult part of the proof is the analysis of term (B). We observe that

$$\partial_R \mathcal{E}^N(s,t) = -\mathcal{E}^N(s,t) \int_s^t \int_{\mathbb{R}^+} \partial_R L(R,r)\, \mathrm{d}\mu_u^N(r)\, \mathrm{d}u.$$

Moreover, $|\mathcal{E}^N(s,t)| \le 1$. Hence, we have

$$\begin{aligned} |(B)| &= \psi(R)\, \mathcal{E}^N(s,t) \left| \int_s^t \int_{\mathbb{R}^+} \partial_R L(R,r)\, \mathrm{d}\mu_u^N(r)\, \mathrm{d}u \right| \left[\int_{\mathbb{R}^+} \widetilde{L}(R,r) \frac{\mathrm{d}\widetilde{\mu}_s(r)}{r} \right] \\ &\le \psi(R) \left[\int_0^t \int_{\mathbb{R}^+} R \left|\partial_R L(R,r)\right| \mathrm{d}\mu_u^N(r)\, \mathrm{d}u \right] \left[\int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{R} \frac{\mathrm{d}\widetilde{\mu}_s(r)}{r} \right]. \end{aligned}$$

Now, we use (P3) in Lemma 3.2 to estimate $R\left|\partial_R L(R,r)\right|$:

$$|(B)| \le \psi(R) \left[\int_0^t \int_{\mathbb{R}^+} \left(\frac{2\sigma}{r} + L(R,r) \right) \mathrm{d}\mu_u^N(r)\, \mathrm{d}u \right] \left[\int_{\mathbb{R}^+} \frac{\widetilde{L}(R,r)}{R} \frac{\mathrm{d}\widetilde{\mu}_s(r)}{r} \right].$$

Finally, we apply (P5) in the Lemma 3.2 to estimate $\frac{\widetilde{L}(R,r)}{R} \le C(\sigma)$ and estimate on $\|\mu_s^N\|_{BL^*,w}$ from Theorem 5.4 (A) to obtain

$$|(B)| \le C_d\, \mathcal{C}_\sigma \left[\int_0^t \int_{\mathbb{R}^+} \left(\frac{2\sigma\, \mathcal{C}_\sigma}{r} + \frac{\widetilde{L}(R,r)}{R\, r} \right) \mathrm{d}\mu_u^N(r)\, \mathrm{d}u \right] \le C_d \int_0^t \int_{\mathbb{R}^+} \frac{\mathrm{d}\mu_u^N(r)}{r}\, \mathrm{d}u \le C_d.$$

□

LEMMA 5.6 Let $\|\psi\|_{BL} \le 1$. Under the notation of the proof of Theorem 5.4 the function defined in (5.16) belongs to $BL(\mathbb{R}^+)$ with constant $C(\sigma)$.

Proof. Recall that L is supported for $|R-r| \le \sigma$ and $|L| \le 2\sigma^2$. Hence, when r is fixed, there are at most $2\sigma/(R_0/N) + 1 = 2\sigma \frac{N}{R_0} + 1 \le (2\sigma+1)\frac{N}{R_0}$ points $x_i = \frac{i}{N} R_0$ in the interval $|R-r| \le \sigma$. It follows that

$$|\mathcal{F}(r)| \le 2\sigma^2 \|\psi\|_\infty \sum_{i=1}^N \frac{R_0}{N} \mathbb{1}_{|x_i - r|} \le 2\sigma^2\,(2\sigma+1).$$

Similarly, as $\psi(R)\,\mathcal{E}^N(s,t)$ does not depend on r, $|\psi(R)\,\mathcal{E}^N(s,t)| \leq 1$ and the map $r \mapsto \widetilde{L}(R,r)$ is in $BL(\mathbb{R}^+)$ with constant $C(\sigma)$, cf. Lemma 3.2 (P2), we have for some r_1 and r_2:

$$|\mathcal{F}(r_1) - \mathcal{F}(r_2)| = \left| \int_{\mathbb{R}^+} \psi(R)\,\mathcal{E}^N(s,t)\,\left(\widetilde{L}(R,r_1) - \widetilde{L}(R,r_2)\right) \mathrm{d}\lambda_N(R) \right|$$
$$\leq \sum_{i=1}^{N} \frac{R_0}{N}\, C(\sigma)\,\left(\mathbb{1}_{|x_i - r_1| \leq \sigma} + \mathbb{1}_{|x_i - r_2| \leq \sigma}\right) |r_1 - r_2| \leq 2\,(2\sigma + 1)\,C(\sigma)\,|r_1 - r_2|.$$

□

6. Convergence result: proof of Theorem 1.1

Let μ_0 be a measure generated by the density $p(r,0) = 4\pi r^2\, n_0(r)$, i.e. $\mu_0(A) = \int_A p(r,0)\,\mathrm{d}r$. Then, μ_0 satisfies Assumption 5.1 and assumptions of Theorem 4.3 because n_0 is bounded and compactly supported, cf. Remark 4.4. In what follows,

- μ_t is the unique measure solution to (1.2) with initial condition μ_0,
- $\mu_t^N = \sum_{i=1}^N m_i(t)\,\delta_{x_i}$ is the solution to the numerical scheme (1.4) with initial condition $\mu_0^N = \sum_{i=1}^N m_i(0)\,\delta_{x_i}$,
- $\widetilde{\mu}_t$ is the unique measure solution to (1.2) with initial condition μ_0^N.

According to Theorem 4.3, we have

$$\left\| \mu_t - \widetilde{\mu}_t \right\|_{BL^*,w} \leq C \left\| \frac{\mu_0 - \mu_0^N}{r \min(1,r)} \right\|_{BL^*}$$

for some constant C depending on data and initial condition μ_0. Now, we observe that if n_0 is supported on $[0,\gamma]$ then

$$\int_{\mathbb{R}^+} \frac{p_0(r)}{r\min(1,r)}\,\mathrm{d}r = \int_{\mathbb{R}^+} \frac{4\pi r^2\, n_0(r)}{r\min(1,r)}\,\mathrm{d}r \leq \|n_0\|_\infty\,\gamma\,\max(1,\gamma) < \infty,$$

where we applied estimate $\frac{r}{\min(1,r)} \leq \max(1,r)$. Hence, we may apply Lemma 2.3 with $f(r) = r\min(1,r)$ to obtain

$$\left\| \mu_t - \widetilde{\mu}_t \right\|_{BL^*,w} \leq C \left\| \frac{\mu_0 - \mu_0^N}{r \min(1,r)} \right\|_{BL^*} \leq C\,\frac{R_0}{N}. \tag{6.1}$$

Moreover, directly from Theorem 5.4 (C), we obtain

$$\left\| \widetilde{\mu}_t - \mu_t^N \right\|_{BL^*,w} \leq C\,\frac{R_0^2}{N} + C\,e^{-R_0}, \tag{6.2}$$

where we chose $M(R) = e^R$ for simplicity (in fact any M from Remark 5.2 can be chosen as initial condition is compactly supported). Combining (6.1) and (6.2), we deduce

$$\left\| \mu_t - \mu_t^N \right\|_{BL^*,w} \leq C\,\frac{R_0}{N} + C\,\frac{R_0^2}{N} + C\,e^{-R_0} \leq C\,\frac{R_0^2}{N} + C\,e^{-R_0}$$

because R_0 is large (say $R_0 \geq 1$). This concludes the proof.

7. Comment on two-dimensional case and consequences on convergence

In this section we briefly discuss the case $d = 2$. This time the change of variables yields the following result.

THEOREM 7.1 (Radial change of coordinates in two dimension). Let $d = 2$ and let $n(x,t)$ be the solution to (1.1) with radially symmetric initial condition $n_0(x)$. Then the radial density $p(R,t)$ defined with

$$p(R,t) = 2\pi R\, n((0,R),t), \qquad p_0(R) = 2\pi R\, n_0((0,R)),$$

satisfies equation

$$\partial_t p(R,t) \;=\; (2\pi R \;-\; p(R,t)) \int_0^\infty L(R,r)\, p(r,t)\,\mathrm{d}r, \tag{7.1}$$

where the radial interaction kernel L is given by

$$L(R,r) = \frac{1}{\pi^2\sigma^2}\left[\frac{\pi}{2} - \arcsin\max\left(\frac{R^2 + r^2 - \sigma^2}{2Rr}, -1\right)\right] \mathbb{1}_{|R-r|\leq\sigma}. \tag{7.2}$$

Proof of Theorem 7.1 is deferred to the end of this section. Here, we briefly discuss how to adapt three-dimensional proof to the two-dimensional case.

First, the resulting kernel $L(R,r)$ cannot be expected to be Lipschitz continuous, even away from $R, r = 0$, because function $x \mapsto \arcsin(x)$ is not Lipschitz (its derivative blows up at $x = \pm 1$). However, it is well-known that $\arcsin(x)$ is $1/2$-Hölder continuous. In other words, it is Lipschitz continuous with respect to the metric $d_{1/2}(x,y) = |x-y|^{1/2}$.

To exploit this fact we use the theory of measure spaces on general metric spaces, cf. Düll *et al.* (2021). Mimicking definitions (2.3)–(2.5), we define

$$BL_{1/2}(\mathbb{R}^+) = \left\{ f : \mathbb{R}^+ \to \mathbb{R} \text{ is continuous and } \|f\|_\infty < \infty, |f|_{1/2} < \infty \right\},$$

where

$$\|f\|_\infty = \sup_{x\in\mathbb{R}^+} |f(x)|, \qquad |f|_{1/2} = \sup_{x\neq y} \frac{|f(x) - f(y)|}{|x-y|^{1/2}}. \tag{7.3}$$

Space $BL_{1/2}(\mathbb{R}^+)$ is equipped with the norm

$$\|f\|_{BL,\,1/2} = \max\left(\|f\|_\infty,\, |f|_{1/2}\right) \leq \|f\|_\infty + |f|_{1/2}. \tag{7.4}$$

Similarly, as in (2.9), we define weighted flat norm:

$$\|\mu\|_{BL^*,1/2,w} := \sup\left\{\int_{\mathbb{R}^+} \frac{\psi(r)}{\sqrt{r}}\,\mathrm{d}\mu(r) : \psi \in BL_{1/2}(\mathbb{R}^+),\, \|\psi\|_{BL,\,1/2} \leq 1\right\}. \tag{7.5}$$

This time we scale with $\sqrt{r}$ rather than r because function $r \mapsto \sqrt{r}$ is 1/2-Hölder continuous, so it will interplay nicely with test functions in $BL_{1/2}(\mathbb{R}^+)$.

Note that the distance between two Dirac masses in the numerical scheme equals R_0/N. By Lemma 2.3 we see that arbitrary measure can be also approximated with finite combinations of Dirac masses with respect to $\|\cdot\|_{BL^*,1/2,w}$ norm with an error of size $R_0^{1/2}/N^{1/2}$. Therefore, in two dimensions, we should expect that the methods of this paper yield estimate

$$\left\|p(\cdot,t) - \mu_t^N\right\|_{BL^*,1/2,w} \leq C\,\frac{R_0}{\sqrt{N}} + C\,e^{-R_0},$$

contrary to (1.5). This is indeed illustrated in the numerical simulations in Section 8.

Proof of Theorem 7.1. The kernel is given by

$$K(r) = \frac{1}{\pi\,\sigma^2}\,\mathbb{1}_{[0,\sigma]}(r). \tag{7.6}$$

Similarly, to the three-dimensional case, we let $p(R,t) = 2\pi R\, n(x,t)$, where $R = |x| = (x_1^2 + x_2^2)^{1/2}$. The convolution $k * n$ is also a radially symmetric function given by

$$\begin{aligned} k * n(x,t) &= k * n((0,R),t) \\ &= \int_{\mathbb{R}^2} K\left(\left((0-y_1)^2 + (R-y_2)^2\right)^{1/2}\right) n((y_1,y_2),t)\,\mathrm{d}y \\ &= \int_{\mathbb{R}^2} K\left(\left(y_1^2 + y_2^2 + R^2 - 2R\,y_2\right)^{1/2}\right) p\left(\left(y_1^2+y_2^2\right)^{1/2}, t\right) \frac{1}{2\pi\sqrt{y_1^2+y_2^2}}\,\mathrm{d}y. \end{aligned} \tag{7.7}$$

To convert (1.1) to polar coordinates, we substitute

$$y_1 = r\cos\alpha, \qquad y_2 = r\sin\alpha, \tag{7.8}$$

where $r > 0$ and $0 \leq \alpha \leq 2\pi$. The Jacobian determinant of the change of variables in (7.8) is equal to r. Using

$$r^2 = y_1^2 + y_2^2, \qquad 2R\,y_2 = 2R\,r\sin\alpha$$

to (7.7), substituting $u = r^2 + R^2 - 2\,R\,r\sin\alpha$ $\left(\text{so that} \sin\alpha = \frac{r^2+R^2-u}{2\,R\,r}\right)$, and using the fact that (7.6) is an indicator function, we obtain

$$\begin{aligned}
&\int_0^\infty \int_0^{2\pi} K\left((r^2 + R^2 - 2R\,r\,\sin\alpha)^{1/2}\right) \frac{1}{2\pi\,r} r\,p(r,t)\,\mathrm{d}\alpha\,\mathrm{d}r \\
&= \frac{2}{2\pi} \int_0^\infty \int_{(R-r)^2}^{(R+r)^2} \frac{K\left(u^{1/2}\right) p(r,t)}{\sqrt{4R^2r^2 - (R^2 + r^2 - u)^2}}\,\mathrm{d}u\,\mathrm{d}r \\
&= \frac{1}{\pi^2\,\sigma^2} \int_{|R-r|\le\sigma} \int_{(R-r)^2}^{\min\{\sigma^2,\,(R+r)^2\}} \frac{p(r,t)}{\sqrt{4R^2r^2 - (R^2 + r^2 - u)^2}}\,\mathrm{d}u\,\mathrm{d}r.
\end{aligned}$$

Again, substituting $w = \frac{R^2+r^2-u}{2Rr}$ and integrating with respect to w, we obtain

$$\frac{1}{\pi^2\,\sigma^2} \int_{|R-r|\le\sigma} \left[\frac{\pi}{2} - \arcsin\max\left(\frac{R^2 + r^2 - \sigma^2}{2Rr}, -1\right)\right] p(r,t)\,\mathrm{d}r.$$

□

8. Simulation results

This section presents the computational results illustrating the theoretical estimation concerning the orders of convergence of the numerical method used to solve (1.2) and (7.1). As the Runge–Kutta method requires higher regularity of the right-hand side, to deal with the resulting ODE system we use the explicit Euler scheme. Data and relevant code for this research work are stored in GitHub: https://github.com/Zuzanna-Szymanska/Non-local-proliferation-model and have been archived within the Zenodo repository (Szymańska *et al.* 2021b).

While investigating the mentioned orders of convergence we assume each time $\Delta t = \Delta r$. We divide simulation time T into $T/\Delta t$ time steps and the spatial domain R_0 into $R_0/\Delta t$ space cells. Then $\mu_t^{N_{\Delta t}}$ denotes the numerical solution obtained for time t, and $N_{\Delta t}$ space cells, where $N_{\Delta t} = R_0/\Delta t$. We define the relative error of the numerical solution $\mu_t^{N_{\Delta t}}$ as the flat norm of the distance between the solution $\mu_t^{N_{\Delta t}}$ and $\mu_t^{N_{\Delta 2t}}$, that is

$$\mathrm{Err}(\Delta t) = \|\mu_t^{N_{\Delta t}} - \mu_t^{N_{\Delta 2t}}\|_{BL^*,w}, \tag{8.1}$$

where the norm is defined by (2.9). Then, the rate of convergence, denoted by q, is given by the following formula

$$q := \lim_{\Delta t\to 0} q_{\Delta t}, \qquad q_{\Delta t} := \frac{\log(\mathrm{Err}(2\Delta t))/(\mathrm{Err}(\Delta t))}{\log 2}. \tag{8.2}$$

In the following computations, flat norm and Wasserstein distance were computed using standard algorithms, cf. Jablonski & Marciniak-Czochra, (2013, Sections 3.1, 3.3) or Düll *et al.* (2021, Chapters 4.2–4.4)

Three-dimensional case. Table 1 presents the obtained relative error and the order of convergence of the numerical scheme applied to solve (1.2). The simulations were conducted on the spatial domain R_0

TABLE 1 *Error computed in flat metric Err (Δt)(8.1) together with corresponding order of convergence (8.2) for the model given by (1.2)*

$\Delta t = \Delta r$	Err (Δt)	$q_{\Delta t}$
$1.5625 \cdot 10^{-5}$	$3.86073194 \cdot 10^{-5}$	–
$3.125 \cdot 10^{-5}$	$7.79035932 \cdot 10^{-5}$	1.0128154842837573
$6.25 \cdot 10^{-5}$	$1.574836435 \cdot 10^{-4}$	1.0154402184761508
$1.25 \cdot 10^{-4}$	$3.259716168 \cdot 10^{-4}$	1.0495443548927024
$2.5 \cdot 10^{-4}$	$6.788816649 \cdot 10^{-4}$	1.0584137711334787
$5.0 \cdot 10^{-4}$	$1.534610347 \cdot 10^{-3}$	1.1766403603675424
$1.0 \cdot 10^{-3}$	$3.775119532 \cdot 10^{-3}$	1.2986499380494803

equal to 2 and smallest $\Delta t = 1.5625 \cdot 10^{-5}$, which gives us $1.28 \cdot 10^5$ mass points for the smallest discretization, whereas the simulation time T was equal to 10. We formulated the initial condition to be the same as the one adopted in our companion paper on modelling cells' proliferation within a solid tumour, see Szymańska *et al.* (2021a) for a precise explanation of the launched formula. In short, we assume that the initial condition is given by

$$p(r, 0) = 4\pi r^2 \left(1 - \left(\frac{r}{\tilde{\sigma}_i}\right)^{\tilde{q}}\right) \mathbb{1}_{[0,\tilde{\sigma}_i]}(r), \tag{8.3}$$

where $\tilde{\sigma}_i = 0.79$ and $\tilde{q} = 13$ are chosen so to match the experimental data we used to estimate parameters of the model. The original model includes an additional parameter describing the proliferation rate. More precisely, instead of (3.2), we consider now

$$L(R, r) = \frac{3\alpha}{16\pi\,\sigma^3} \frac{\min\{(R+r)^2, \sigma^2\} - \min\{(R-r)^2, \sigma^2\}}{R\,r}, \tag{8.4}$$

where both α and σ, together with σ_i from the initial condition, were subjects of parameter estimation (Szymańska *et al.*, 2021a). Within the present computations, $\alpha = 0.5$ and $\sigma = 0.04$ are chosen to get solutions sufficiently distant from the initial condition to investigate the orders of convergence, rather than to meet the experimental data.

Two-dimensional case. Computation of the flat metric with respect to Hölder metric is slightly difficult. Therefore, we introduce the following distance on $\mathcal{M}(\mathbb{R}^+)$:

$$\rho\big(\mu_1, \mu_2\big) = \min\Big\{M_{\mu_1}, M_{\mu_2}\Big\} W_1\big(\tilde{\mu}_1, \tilde{\mu}_2\big) + \Big|M_{\mu_1} - M_{\mu_2}\Big|, \tag{8.5}$$

where $M_{\mu_i} = \int_{\mathbb{R}^+} \mathrm{d}\mu_i \neq 0$, $\tilde{\mu}_i = \mu_i / M_{\mu_i}$ and W_1 is the usual Wasserstein distance with respect to $\frac{1}{2}$-Hölder metric, i.e.

$$W_1\big(\tilde{\mu}_1, \tilde{\mu}_2\big) = \sup\left\{ \int_{\mathbb{R}^+} \psi(r)\,\mathrm{d}(\mu_1 - \mu_2)(r) \quad \Big| \quad \psi : \mathbb{R}^+ \to \mathbb{R}, |\psi|_{1/2} \le 1 \right\}.$$

It is well-known that for measures defined on bounded intervals of $\mathbb{R}^+$ metric, ρ is equivalent with the flat norm (Carrillo *et al.*, 2014, 2019). In the following computations we use ρ because there is a simple

TABLE 2 *Error computed in metric Err (Δt)(8.6) together with corresponding order of convergence (8.2) for the model given by (7.1)*

$\Delta t = \Delta r$	Err (Δt)	$q_{\Delta t}$
$1.5625 \cdot 10^{-5}$	$7.458465570038538 \cdot 10^{-3}$	–
$3.125 \cdot 10^{-5}$	$1.0997423574488038 \cdot 10^{-2}$	0.5602148149156739
$6.25 \cdot 10^{-5}$	$1.643673194250337 \cdot 10^{-2}$	0.5797579061447363
$1.25 \cdot 10^{-4}$	$2.510571793647852 \cdot 10^{-2}$	0.6110925001107623
$2.5 \cdot 10^{-4}$	$3.908330914430527 \cdot 10^{-2}$	0.6385366423383074
$5.0 \cdot 10^{-4}$	$6.313477587243083 \cdot 10^{-2}$	0.691882264852459
$1.0 \cdot 10^{-3}$	$1.0560403857421896 \cdot 10^{-1}$	0.7421582142026246

linear algorithm to compute W_1, cf. Jablonski & Marciniak-Czochra, (2013, Sections 3.1, 3.3) or Düll *et al*. (2021, Chapters 4.2–4.4).

We define the relative error as the distance between weighted solutions $\mu_t^{N_{\Delta t}}$ and $\mu_t^{N_{\Delta 2t}}$:

$$\mathrm{Err}(\Delta t) = \rho\left(\frac{\mu_t^{N_{\Delta t}}}{\sqrt{r}}, \frac{\mu_t^{N_{\Delta 2t}}}{\sqrt{r}}\right). \tag{8.6}$$

Here, $\frac{\mu_t^{N_{\Delta t}}}{\sqrt{r}}$ is a weighted measure as in (2.6)–(2.7) defined with the formula

$$\frac{\mu_t^{N_{\Delta t}}}{\sqrt{r}}(A) = \int_A \frac{1}{\sqrt{r}}\,\mathrm{d}\mu_t^{N_{\Delta t}}(r),$$

and similarly for $\frac{\mu_t^{N_{\Delta 2t}}}{\sqrt{r}}$. Then, the order of convergence is computed as in (8.2).

Finally, the initial condition for the two-dimensional case is similar to (8.3) with the only adjustment of considered dimension, i.e. term $2\pi r$ instead of $4\pi r^2$. Analogously to three-dimensional case now instead of (7.2), we consider

$$L(R, r) = \frac{\alpha}{\pi^2\sigma^2}\left[\frac{\pi}{2} - \arcsin\max\left(\frac{R^2 + r^2 - \sigma^2}{2Rr}, -1\right)\right]\mathbb{1}_{|R-r|\le\sigma}. \tag{8.7}$$

Now, Table 2 presents the obtained relative error and the order of convergence of the numerical scheme applied to solve (7.1). Similarly to the three-dimensional case, the presented simulations were conducted on the spatial domain R_0 equal to 2 and smallest $\Delta t = 1.5625 \cdot 10^{-5}$, which gives us $1.28 \cdot 10^5$ mass points for the smallest discretization, whereas the simulation time T was equal to 10.

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