Particle dynamics in bounded domains

学位論文要旨

Particle dynamics in bounded domains

有界領域における粒子運動

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1 Summary

We consider the dynamics of interacting particle systems where particles are confined to a bounded domain Ω. To control the particles not to escape the domain, there are many boundary rules to particle on $\partial\Omega$. But under these boundary rules, rigorous solution concept for particle trajectory is missing. Our aim is therefore to establish a satisfactory analytical framework for particle dynamics where particles are confined to a bounded, possibly nonconvex domain Ω. We consider two problems in this thesis, one is a first order ODE system, when particles hit the boundary, we consider an instant change in velocity. The other one is a second order ODE system, we consider collisions with the boundary are described as purely elastic collisions. This provide a theoretical basis for the boundary conditions of particle methods.

2 First order discontinuous ODEs

Let Ω be a bounded domain in $\mathbb{R}^m$ with C^2 boundary $\partial\Omega$. We denote the outward unit normal vector on $\partial\Omega$ by ν.

We consider n particles $x_1, \dots, x_n$ in $\overline{\Omega}$. We put $X := \{x_i\}_{i=1}^n \in \overline{\Omega}^n \subset (\mathbb{R}^m)^n$ as the array of the particle's positions. On $(\mathbb{R}^m)^n$ we define the norm

$$\|X\| := \max_{1\le i\le n} |x_i|,$$

where $|x_i|$ is the Euclidean distance in $\mathbb{R}^m$.

Next we introduce the dynamics of the particle system. We denote by $X(t) = \{x_i(t)\}_{i=1}^n$ the particle positions in time, and by $\dot{x}_i(t) = \dfrac{dx_i}{dt}(t)$ their velocity. We prescribe the velocity of any particle $x_i(t)$ depending on whether $x_i(t)$ is in the interior or at the boundary of Ω. If $x_i(t) \in \Omega$, then its velocity is given by the force $F_i(t, X(t))$, where

$$F_i \in C([0,T]\times\overline{\Omega}^n;\mathbb{R}^m) \quad (i = 1,\dots,n). \tag{2.1}$$

In some cases, we impose the following hypothesis on Lipschitz continuity of F_i: there exists an $L > 0$ such that

$$|F_i(t,X) - F_i(t,Y)| \le L\|X - Y\| \quad (t\in[0,T],\ X,Y\in(\mathbb{R}^m)^n,\ i = 1,\dots,n). \tag{2.2}$$

If $x_i(t) \in \partial\Omega$, then we prescribe a different rule. If the force $F_i(t, X(t))$ acting on $x_i(t)$ is directed to the interior of Ω, then we prescribe its velocity by $F_i(t, X(t))$. Otherwise, we project $F_i(t, X(t))$ onto the tangent plane of $\partial\Omega$ at $x_i(t)$. To define this rule mathematically, we put

$$P : \overline{\Omega}\times\mathbb{R}^m \to \mathbb{R}^m, \quad P(x,f) := \begin{cases} f - \big(f\cdot\nu(x)\big)\nu(x) & (x\in\partial\Omega, f\cdot\nu(x) > 0), \\ f & \text{otherwise}, \end{cases} \tag{2.3}$$

and prescribe the velocity of $x_i(t)$ as $P(x_i(t), F_i(t, X))$. For convenience, we set

$$H_i : [0,T]\times\overline{\Omega}^n \to \mathbb{R}^m, \quad H_i\big(t,X\big) := P\big(x_i, F_i(t,X)\big) \quad (t\in[0,T], X = \{x_i\}_{i=1}^n \in \overline{\Omega}^n).$$

To summarise the dynamics of the particles, we introduce the following problem:

Problem 2.1. *Let $n \in \mathbb{N}$ and $T > 0$. For each $i = 1, \dots, n$, let F_i be as in (2.1), and $x_i^\circ \in \Omega$. Find a solution $X(t) = \{x_i(t)\}_{i=1}^n$ to*

$$\begin{cases} \dot{x}_i(t) = H_i\big(t, X(t)\big) & (t \in (0,T)), \\ x_i(0) = x_i^\circ. \end{cases}$$

for $i = 1, \dots, n$.

Since H_i is discontinuous, we do not expect solutions to Problem 2.1 to be C^1 in time. Instead, we consider mild solutions:

Definition 2.2. *We say that $X(t) = \{x_i(t)\}_{i=1}^n$ is a (mild) solution to Problem 2.1 if for all $i \in \{1, \dots, n\}$, $x_i \in C^0([0,T]; \mathbb{R}^m)$, and $x_i(t) \in \overline{\Omega}$ for all $t \in [0,T]$ and satisfies*

$$x_i(t) = x_i^\circ + \int_0^t H_i\big(s, X(s)\big) ds \quad (t \in [0,T]).$$

The following proposition gives a convenient characterisation of mild solutions. Since the proof is elementary, we omit it.

Proposition 2.3. *For Problem 2.1, $X(t) = \{x_i(t)\}_{i=1}^n$ is a mild solution if and only if*

$$\begin{cases} x_i \in \mathrm{Lip}([0,T]; \mathbb{R}^m) \\ \dot{x}_i(t) = H_i(t, X(t)) \quad \big(a.e.\ t \in [0,T]\big) \\ x_i(0) = x_i^\circ. \end{cases}$$

Our main result is the following theorem, which grants the existence and uniqueness of mild solutions to Problem 2.1:

Theorem 2.4. *Let $T > 0$ and $X^\circ \in \overline{\Omega}^n$. If F_i satisfies (2.1), then there exists a solution to Problem 2.1. Moreover, if F_i satisfies the Lipschitz condition (2.2), then the solution is unique.*

We construct an approximation of Problem 2.1 by replacing the "one-sided projection" and the condition that $x_i \in \overline{\Omega}$ by a force field outside of Ω which pushes a particle back inside Ω. This force field is given by $-kd\nabla d : \mathbb{R}^m \to \mathbb{R}^m$, where $k \in \mathbb{N}$ is a (large) parameter which dictates the strength of the force Since particles may leave Ω, we need to extend the domain of F_i beyond $\overline{\Omega}^n$. By (2.1), we may extend it to $(\mathbb{R}^m)^n$ as a continuous and bounded function. In the following, we take any such extension, and denote it simply by

$$F_i \in C_b([0,T] \times (\mathbb{R}^m)^n; \mathbb{R}^m) \quad (i = 1, \dots, n). \tag{2.4}$$

We define

$$\mathrm{dist}(x, K) := \inf_{y \in K} |x - y|,$$
$$N^\varepsilon(K) := \{x \in \mathbb{R}^m \ ; \ \mathrm{dist}(x, K) < \varepsilon\}.$$

For the domain Ω, we define the distance function d with respect to Ω as

$$d : \mathbb{R}^m \to [0, \infty) \quad d(x) := \mathrm{dist}(x, \overline{\Omega})$$

Problem 2.5. *Let $n, k \in \mathbb{N}$ and $T > 0$. For each $i = 1, \dots, n$, let F_i be as in (2.4), and $x_i^\circ \in \Omega$. Find a solution $X^k(t) = \{x_i^k(t)\}_{i=1}^n$ to*

$$\begin{cases} \dot{x}_i^k(t) = F_i(t, X^k(t)) - k(d\nabla d)(x_i^k(t)) \quad (t \in (0,T)), \\ x_i^k(0) = x_i^\circ, \end{cases} \tag{2.5}$$

for $i = 1, \dots, n$.

Figure 1 illustrates how solutions to Problem 2.5 approximate the projection in a more regular fashion. Then, we have the following lemma.

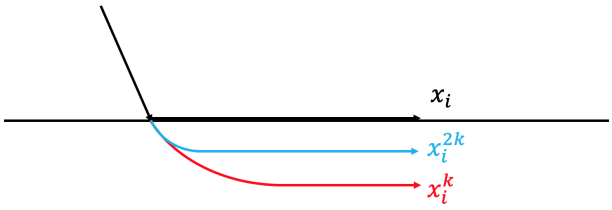

Figure 1: Sketch of the trajectory of a solution x_i to Problem 2.1 and two trajectories of solutions to the approximate Problem 2.5.

Lemma 2.6. *For all k large enough, there exists a classical solution $X^k \in C^1([0,T]; \mathbb{R}^m)$ to Problem 2.5. Moreover, there exists a constant $C > 0$ such that for all k large enough and for any classical solution X^k:*

(i) $\|d(x_i^k)\|_{C([0,T])} \leq C/k$ *for* $i = 1, \dots, n$,

(ii) $\|\dot{X}^k\|_{C([0,T])} \leq C$,

To prove the existence statement of Theorem 2.4. Given T and X° as in Problem 2.1, let X^k be a corresponding solution to Problem 2.5 for each k large enough. The following Lemma specifies compactness properties for the sequence X^k, and shows that any limit point satisfies Definition 2.2.

Lemma 2.7. *Let $\{X^k\}$ be as above. Then, there exists an $X \in W^{1,\infty}(0,T; (\mathbb{R}^m)^n) \cap C^0([0,T]; \overline{\Omega}^n)$ such that*

$$\begin{cases} x_i^k \to x_i & \text{strongly in } C^0([0,T]; \mathbb{R}^m), \\ \dot{x}_i^k \rightharpoonup \dot{x}_i & \text{weakly-}* \text{ in } L^\infty(0,T; \mathbb{R}^m), \end{cases} \tag{2.6}$$

for $i = 1, \dots, n$ as $k \to \infty$.

Let X be given by Lemma 2.7. In the remainder of the proof we pass to the limit $k \to \infty$ in the weak form of (2.5) in order to show that X satisfies the second of the three conditions in Proposition 2.3. Let $\psi \in C_0^\infty((0,T); \mathbb{R}^m)$ be a test function. We fix $i \in \{1, \dots, n\}$ and define the open set $I_k := \{t \in$

$[0,T]\ ;\ x_i^k(t) \notin \overline{\Omega}\}$. Starting from the weak form of (2.5), we obtain

$$\begin{aligned}\int_0^T (\dot{x}_i^k(t) - F_i(t, X^k(t))) \cdot \psi(t) dt &= -\int_0^T k(d\nabla d)(x_i^k(t)) \cdot \psi(t) dt \\ &= -\int_{I_k} k d(x_i^k(t)) \nabla d(x_i^k(t)) \cdot \psi(t) dt \\ &= \int_{I_k} \big(\frac{d}{dt} d(x_i^k(t)) - \nabla d(x_i^k(t)) \cdot F_i(t, X^k(t))\big) \nabla d(x_i^k(t)) \cdot \psi(t) dt \\ &= A_k - B_k,\end{aligned} \tag{2.7}$$

where

$$\begin{aligned}A_k &= \int_{I_k} \big(\frac{d}{dt} d(x_i^k(t))\big) \nabla d(x_i^k(t)) \cdot \psi(t) dt, \\ B_k &= \int_{I_k} \big(\nabla d(x_i^k(t)) \cdot F_i(t, X^k(t))\big) \big(\nabla d(x_i^k(t)) \cdot \psi(t)\big) dt.\end{aligned}$$

Then, we have

$$\lim_{k\to\infty} A_k = 0. \tag{2.8}$$

We define

$$\chi_{\partial\Omega}(t) = \begin{cases} 1 & x_i(t) \in \partial\Omega \\ 0 & x_i(t) \in \Omega, \end{cases}$$

we have the following lemma.

Lemma 2.8. *There exists $\overline{\chi} \in L^\infty(0,T;[0,1])$ such that*

$$\lim_{k\to\infty} B_k = \int_0^T \big(\nu(x_i(t)) \cdot F_i(t, X(t))\big)_+ \big(\nu(x_i(t)) \cdot \psi(t)\big) \overline{\chi}(t) \chi_{\partial\Omega}(t) dt$$

Then, by using co-area formula, we can obtain

$$\dot{x}_i(t) = F_i(t) - \big(\nu(x_i(t)) \cdot F_i(t)\big)_+ \nu(x_i(t)) \chi_{\partial\Omega}(t) = H_i(t, X(t)) \quad \text{a.e. } t \in [0,T].$$

We prove the uniqueness statement of Theorem 2.4. We suppose that F_i satisfies the Lipschitz condition (2.2). Let $T > 0$ and $X^\circ \in \overline{\Omega}^n$ be given, and let $X(t) = \{x_i(t)\}_{i=1}^n$ and $Y(t) = \{y_i(t)\}_{i=1}^n$ be two mild solutions of Problem 2.1 subject to the initial condition $Y^\circ = X^\circ$.

We prove uniqueness by applying gronwall inequality. With this aim (recalling that X, Y are Lipschitz continuous we set

$$J_i(t) := \frac{d}{dt}\Big(\frac{1}{2}|x_i(t) - y_i(t)|^2\Big)$$

for $i \in \{1, \dots, n\}$ and a.e. $t \in (0,T)$. The following lemma provides a sufficient bound on $J_i(t)$.

Lemma 2.9. *There exists a constant $C > 0$ independent of X, Y such that*

$$J_i(t) \le C\|X(t) - Y(t)\|^2 \quad (i \in \{1, \dots, n\},\ \textit{a.e. } t \in [0,T]).$$

Then, we have the following theorem

Theorem 2.10 (Approximation theorem)**.** *If F satisfies* (2.1) *and the Lipschitz condition* (2.2)*, the solution $X^k(t)$ of Problem 2.5 is unique for each $k > \|F\|_\infty/\varepsilon$ and it uniformly converges to the unique solution $X(t)$ of Problem 2.1 on $[0,T]$ as $k \to \infty$.*

3 Second order discontinuous ODEs

Let Ω be a bounded domain in $\mathbb{R}^m$ with C^3 boundary $\partial\Omega$. As above in Section 1, we denote the outward unit normal vector on $\partial\Omega$ by ν and consider n particles $x_1, \dots, x_n$ in $\overline{\Omega}$. We put $X := \{x_i\}_{i=1}^n \in \overline{\Omega}^n \subset (\mathbb{R}^m)^n$ as the array of the particle's positions. On $(\mathbb{R}^m)^n$ we define the norm

$$\|X\| := \max_{1\le i\le n} |x_i|,$$

where $|x_i|$ is the Euclidean distance in $\mathbb{R}^m$. We also denote by $X(t) = \{x_i(t)\}_{i=1}^n$ the particle positions in time.

Let us fix on a certain particle x_i with $i \in \{1, \dots, n\}$ for the moment. The acceleration $\ddot{x}_i$ of this particle is given by the force $F_i(t, X(t))$, where F_i satisfies (2.1). Here and henceforth, for any function $f \in C(K; \mathbb{R}^m)$ for some compact $K \subset \mathbb{R}^\ell$ we define the norm

$$\|f\|_{C(K)} := \max_{y\in K} |f(y)|,$$

which we abbreviate by $\|f\|_\infty$ if the domain of f is clear from the context. In some cases, we impose that F_i is Lipschitz continuous in X as in (2.2). If x_i is at the boundary $\partial\Omega$, then we impose the following "reflection rule":

$$\frac{d^+x_i}{dt}(t) = \frac{d^-x_i}{dt}(t) - 2\left(\frac{d^-x_i}{dt}(t)\cdot\nu(x_i(t))\right)\nu(x_i(t)). \tag{3.1}$$

Here,

$$\frac{d^\pm}{dt}x_i(t) := \lim_{h\to 0+}\frac{x_i(t\pm h) - x_i(t)}{\pm h} \tag{3.2}$$

denote the left- and right-derivatives.

Problem 3.1. *Let $n \in \mathbb{N}$ and $T > 0$. For each $i = 1, \dots, n$, let F_i be as in (2.1), $x_i^\circ \in \Omega$ and $v_i^\circ \in \mathbb{R}^m$. Find a solution $X(t) = \{x_i(t)\}_{i=1}^n$ to*

$$\begin{cases} \ddot{x}_i(t) = F_i(t, X(t)) + \text{"reflection rule (3.1) on } \partial\Omega\text{"} \quad (t \in (0,T)), \\ x_i(0) = x_i^\circ, \\ \dfrac{dx_i}{dt}(0) = v_i^\circ \end{cases} \tag{3.3}$$

for $i = 1, \dots, n$.

Since the reflection rule results typically in discontinuous velocities, classical solutions to Problem 3.1 will not exist in general. Therefore, we introduce a weak notion of solutions in Definition 3.2. To define it, we set $\mathcal{M}_+((0,T))$ as the space of finite, non-negative Borel measures on $(0,T)$.

Definition 3.2. *We say that $X(t) = \{x_i(t)\}_{i=1}^n$ is a solution to Problem 3.1 if for all $i \in \{1, \dots, n\}$, x_i satisfies*

(i)

$$\begin{aligned} x_i &\in W^{1,\infty}(0,T;\mathbb{R}^m), \\ x_i(t) &\in \overline{\Omega} \qquad (t \in [0,T]), \\ \dot{x}_i &\in BV(0,T;\mathbb{R}^m), \\ x_i(0) = x_i^\circ, &\quad \frac{d^+x_i}{dt}(0) = v_i^\circ. \end{aligned}$$

(ii) Let $I^i_{\partial\Omega} := \{t \in [0,T]\ ;\ x_i(t) \in \partial\Omega\}$. *There exists* $\rho_i \in \mathcal{M}_+((0,T))$ *with supp* $\rho_i \subset I^i_{\partial\Omega}$ *such that in the sense of distributions,*

$$\ddot{x}_i(t) = F_i(t, X(t)) - \rho_i(t)\nu(x_i(t)),$$

i.e., for any test function $\psi \in C_0^\infty(0,T;\mathbb{R}^m)$,

$$-\int_0^T \dot{x}_i(t)\cdot\dot{\psi}(t)dt = \int_0^T F_i(t,X(t))\cdot\psi(t)dt - \int_{I^i_{\partial\Omega}} \nu(x_i(t))\cdot\psi(t)d\rho_i(t). \tag{3.4}$$

(iii) x_i *satisfies the reflection rule* (3.1) *for all* $t \in I^i_{\partial\Omega}$.

Our main results are the following theorems. They guarantee global existence and local uniqueness of the solutions to Problem 3.1 defined in 3.2.

Theorem 3.3. *Let* $T > 0$, $X^\circ := \{x_i^\circ\}_{i=1}^n \in \Omega^n$ *and* $V^\circ := \{v_i^\circ\}_{i=1}^n \in (\mathbb{R}^m)^n$. *If* F_i *satisfies* (2.1), *then there exists a solution* X *as in Definition 3.2 to Problem 3.1.*

Theorem 3.4. *Given the setting of Theorem 3.3, let* X *be a solution to Problem 3.1, and set*

$$T_0 := \min_{1\le i\le n} \inf\{t \in I^i_{\partial\Omega}\ ;\ \dot{x}_i(t-)\cdot\nu(x_i(t)) = 0\}.$$

If F_i *satisfies* (2.2), *then any solution* Y *to Problem 3.1 coincides with* X *at least up to* T_0, *i.e.,* $Y|_{[0,T_0]} = X|_{[0,T_0]}$.

We construct an approximation of Problem 3.1 by replacing the reflection rule and the condition that $x_i \in \overline{\Omega}$ by a force field outside of Ω which pushes a particle back inside Ω. This force field is given by $-kd\nabla d : \mathbb{R}^m \to \mathbb{R}^m$, where $k \in \mathbb{N}$ is a (large) parameter which dictates the strength of the force. As above in Section 1, since particles may leave Ω, we need to extend the domain of F_i beyond $\overline{\Omega}^n$ as (2.4).

Problem 3.5. *Let* $k \in \mathbb{N}$ *and* $T > 0$. *For* $i = 1,\dots,n$, *let* F_i *be as in* (2.4), *and let* $x_i^\circ \in \Omega$, $v_i^\circ \in \mathbb{R}^m$. *Find a solution* $X^k(t) = \{x_i^k(t)\}_{i=1}^n$ *to*

$$\begin{cases} \ddot{x}_i^k(t) = F_i(t, X^k(t)) - k(d\nabla d)(x_i^k(t)) & (t \in (0,T)), \\ x_i^k(0) = x_i^\circ, \\ \dfrac{dx_i^k}{dt}(0) = v_i^\circ \end{cases} \tag{3.5}$$

for $i = 1,\dots,n$.

Figure 2 illustrates how solutions to Problem 3.5 approximate the reflection in a more regular fashion.

For a continuous solution X^k to Problem 3.5, we set

$$I^{i,k} := \left\{t \in [0,T]\ ;\ x_i^k(t) \notin \overline{\Omega}\right\} \qquad (i = 1,\dots,n)$$

as the set of times at which particle x_i^k is outside of $\overline{\Omega}$. The following lemma provides the global existence of classical solutions to Problem 3.5. It also lists several bounds on such solutions.

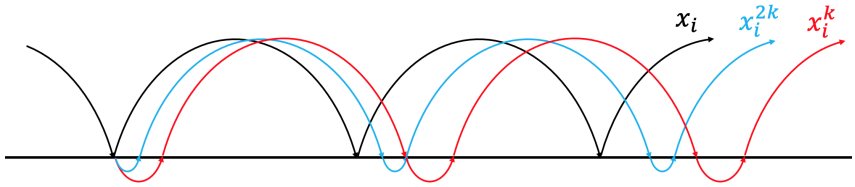

Figure 2: Sketch of the trajectory of a solution x_i to Problem 3.1 and two trajectories of solutions to the approximate Problem 3.5.

Lemma 3.6. *For all k large enough, there exists a classical solution $X^k \in C^2([0,T];\mathbb{R}^m)$ to Problem 3.5. Moreover, there exists a constant $C > 0$ such that for all k large enough and for any classical solution X^k:*

(i) $\|d(x_i^k)\|_{C([0,T])} \leq C/\sqrt{k}$ *for* $i = 1, \dots, n$,

(ii) $\|\dot{X}^k\|_{C([0,T])} \leq C$,

(iii) $\|\ddot{X}^k\|_{L^1(0,T)} \leq C$,

(iv) $\|(d\nabla d)(x_i^k)\|_{L^1(0,T)} \leq C/k$ *for* $i = 1, \dots, n$,

(v) $\|\ddot{x}_i^k\|_{C([0,T]\setminus I^{i,k})} \leq C$ *for* $i = 1, \dots, n$.

Construction of X as in Definition 3.2(i) First we construct a candidate solution X. Given T, x_i°, v_i° as in Problem 3.1, let X^k be a corresponding solution to Problem 3.5 for each k large enough. The following Lemma specifies compactness properties for the sequence $\{X^k\}$, and shows that any limit point satisfies Definition 3.2(i).

Lemma 3.7. *Let $\{X^k\}$ be as above. Then, there exists an X which satisfies Definition 3.2(i) such that*

$$\begin{cases} X^k \to X & \text{in } C^0([0,T];(\mathbb{R}^m)^n), \\ \dot{X}^k \to \dot{X} & \text{in } L^p(0,T;(\mathbb{R}^m)^n) \qquad (p \in [1,\infty)) \end{cases} \tag{3.6}$$

as $k \to \infty$.

X satisfies Definition 3.2(ii) Let X be given by Lemma 3.7, and take $i \in \{1, \dots, n\}$ arbitrary. In the following we prove that x_i satisfies Definition 3.2(ii) for some $\rho_i \in \mathcal{M}_+((0,T))$ with $\operatorname{supp}\rho_i \subset I^i_{\partial\Omega}$ (defined in Definition 3.2(ii)). With this aim, let $\psi \in C_0^\infty(0,T;\mathbb{R}^m)$ be a test function, and note that x_i^k satisfies

$$\int_0^T (-\ddot{x}_i^k + F_i(t, X^k(t))) \cdot \psi(t) dt = \int_0^T k(d\nabla d)(x_i^k(t)) \cdot \psi(t) dt =: A_i^k.$$

With Lemma 3.7 and the continuity of F_i we pass to the limit $k \to \infty$ in the left-hand side. This yields

$$\begin{aligned}\lim_{k\to\infty}\int_0^T (-\ddot{x}_i^k + F_i(t, X^k(t))) \cdot \psi(t) dt &= \lim_{k\to\infty}\left(\int_0^T (\dot{x}_i^k(t) \cdot \dot{\psi}(t) + F_i(t, X^k(t)) \cdot \psi(t)) dt\right) \\ &= \int_0^T (\dot{x}_i(t) \cdot \dot{\psi}(t) + F_i(t, X(t)) \cdot \psi(t)) dt.\end{aligned}$$

And we have the following lemma.

Lemma 3.8.

$$\lim_{k\to\infty} A_i^k = \int_0^T \nu(x_i(t)) \cdot \psi(t) d\rho_i(t) \tag{3.7}$$

for some $\rho_i \in \mathcal{M}_+((0,T))$ *with* $\operatorname{supp}\rho_i \subset I^i_{\partial\Omega}$.

X **satisfies Definition 3.2(iii)** For arbitrary $i \in \{1, \dots, n\}$ and $t_0 \in I^i_{\partial\Omega}$ (defined in Definition 3.2(ii)), we proved that x_i satisfies the reflection rule (3.1) at $t = t_0$, which completes the proof of Theorem 3.3.

Next, we prove local uniqueness of solutions to Problem 3.1 as stated in Theorem 3.4. In addition, we give a counterexample to global-in-time uniqueness. Let X, Y be two solutions to Problem 3.1 and let T_0 be as in Theorem 3.4. We prove Theorem 3.4 by contradiction; suppose that there exists a $T_1 \in [0, T_0)$ and an $i \in \{1, \dots, n\}$ such that for some decreasing sequence $t_\ell \downarrow T_1$ as $\ell \to \infty$ there holds

$$\begin{cases} X(t) = Y(t) & (0 \le t \le T_1), \\ x_i(t_\ell) \ne y_i(t_\ell) & (\ell = 1, 2, \dots). \end{cases} \tag{3.8}$$

We split two cases:

Case 1: $x_i(T_1) \in \Omega$. Let $\delta > 0$ such that the ball $B_\delta(x_i(T_1))$ is contained in Ω. Since x_i and y_i are continuous, there exists $\eta > 0$ such that $x_i(t), y_i(t) \in B_\delta(x_i(T_1)) \subset \Omega$ for all $t \in [T_1, T_1 + \eta)$, and thus $I^i_{\partial\Omega} \cap [T_1, T_1 + \eta) = \emptyset$. Then, since $\operatorname{supp}\rho_i \subset I^i_{\partial\Omega}$, there exists a unique classical solution for Problem 3.1 on $(T_1, T_1 + \eta)$ from the Lipschitz condition (2.2). This contradicts (3.8).

Case 2: $x_i(T_1) \in \partial\Omega$ with $\alpha := \dot{x}_i(T_1-) \cdot \nu(x_i(T_1)) > 0$. From (3.8) we note that $\alpha = \dot{y}_i(T_1-) \cdot \nu(y_i(T_1))$. Then, from the reflection rule (3.1), we obtain $\dot{x}_i(T_1+) \cdot \nu(x_i(T_1)) = \dot{y}_i(T_1+) \cdot \nu(y_i(T_1)) = -\alpha < 0$. Hence, there exists an $\eta > 0$ such that $x_i(t), y_i(t) \in \Omega$ for all $T_1 < t < T_1 + \eta$. Then, a similar argument as in Case 1 yields a contradiction with (3.8).

Our counterexample is set on the one-dimensional ($m = 1$) halfline $\Omega := \{x \in \mathbb{R} \ ; \ x > 0\}$ with $x^\circ = x_1^\circ = 0$ and $v^\circ = v_1^\circ = 0$ as initial conditions. This initial condition corresponds in the setting of Theorem 3.4 to $T_0 = 0$. While this initial condition is technically not allowed in Theorem 3.3, it can easily be obtained by having the particle start inside Ω at $t = 0$, choose an F so that the particle enters $\partial\Omega$ at 0 speed at $t = 1/2$, keep the particle on the boundary until $t = 1$, and then shift time backwards by 1 unit. For any given $L \in \mathbb{N}$, we will construct a function $F(t) := F_1(t, x(t))$ of class C^L which is non-positive (this is in line with the setting of the tennis player). For any such F, the 0-function is a solution according to Definition 3.2 (in this case, the density of $\rho = \rho_1$ is $-F(t)$), and thus it remains to construct a non-zero solution.

Before constructing an F which results in a non-zero solution, we remark that our one-dimensional setup is not restrictive. Indeed, simply by adding a second dimension to our current setup, Ω becomes the halfplane, and x_2 can be considered as constant. Our example will also trivially extend to the case in which $v_2^\circ \neq 0$, in which case $x_2(t)$ changes linearly in time. In this case, F need not explicitly depend on time, and instead dependence on $x_2(t)$ suffices. More generally, our example can be extended to higher dimensions and a curved boundary $\partial\Omega$.

Next we construct F in our one-dimensional setting such that Definition 3.2 has a non-zero solution $x(t)$. We do this by tying together rescaled and translated versions of an auxiliary problem where a particle with position $z(t)$ only bounces at the start and end time. Our goal in this auxiliary problem is that the speed of impact $-v_1$ at the end time 1 is larger than the initial speed v_0 at $t = 0$, i.e., $v_1 - v_0 > 0$.

To reach this goal, let $f \in C_0^\infty(0,1)$ with $f(t) \geq 0$ satisfy

$$\int_0^1 (2s-1)\, f(s)ds > 0. \tag{3.9}$$

For $v_0 > 0$ to be chosen later, let z be the solution to

$$\begin{cases} z''(t) = -f(t), \\ z(0) = 0, \\ z'(0) = v_0. \end{cases}$$

It is easy to see that $z(t) = v_0 t - \int_0^t (t-s)f(s)ds$. Next we choose v_0 such that the particle hits the boundary again at $t = 1$, i.e., such that $z(1) = 0$. This yields

$$v_0 = \int_0^1 (1-s)f(s)ds$$

We then find that

$$v_1 = -z'(1) = \int_0^1 sf(s)ds.$$

Finally, to test the requirement $v_1 - v_0 > 0$, we compute

$$v_1 - v_0 = \int_0^1 (2s-1)\, f(s)ds,$$

and observe from 3.9 that this value is indeed positive.

Next we rescale the auxiliary problem. For $a, b > 0$ to be chosen later, let

$$y(t) := bz\left(\frac{t}{a}\right) \qquad (t \in [0,a]).$$

Then, y satisfies

$$\begin{cases} y''(t) = -\dfrac{b}{a^2} f\left(\dfrac{t}{a}\right), \\ y(0) = y(a) = 0, \\ y'(0) = \dfrac{b}{a} v_0, \\ y'(a) = -\dfrac{b}{a} v_1. \end{cases}$$

Next we tie the rescaled problems together by shifting them in space. Figure 3 illustrates the corresponding construction. The reflection rule dictates that minus the velocity at the end time of the scaled auxiliary problem to the left has to equal the velocity at initial time of the scaled auxiliary problem to the right, i.e., $v_0 = \frac{b}{a} v_1$. This requires $b < a < 1$. The shifted time interval of the n-th bounce to the left is given by $I_n := (\frac{a^{n+1}}{1-a}, \frac{a^n}{1-a})$. The resulting function F is

$$F(t) = \begin{cases} -\left(\frac{b}{a^2}\right)^n f\left(\left(t - \frac{a^{n+1}}{1-a}\right) a^{-n}\right) & (t \in I_n, n \in \mathbb{Z}), \\ 0 & \text{otherwise}, \end{cases} \tag{3.10}$$

where we allow for $t < 0$. For this non-positive F, a non-zero solution x to Problem (3.1) is

$$x(t) = \begin{cases} b^n z\left(\left(t - \frac{a^{n+1}}{1-a}\right) a^{-n}\right) & (t \in I_n, n \in \mathbb{Z}), \\ 0 & \text{otherwise}, \end{cases} \tag{3.11}$$

which we also extend by 0 for $t < 0$.

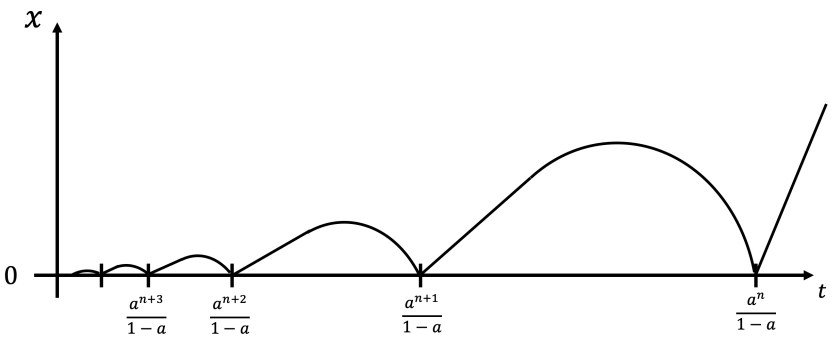

Figure 3: Sketch of the non-zero solution $x(t)$.

We can check that x is indeed a solution to Problem 3.1.

令和３ 年１月 27 日

学位論文審査報告書（甲）

１．学位論文題目（外国語の場合は和訳を付けること。）

Particle dynamics in bounded domains （有界領域における粒子運動）

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３．審査結果の要旨（600～650 字）

楊振興君は、2016 年４月に数物科学専攻博士前期課程に入学し、2018 年４月に同博士後期課程に進学した。研究テーマは、有界領域内の多粒子運動を記述する微分方程式の数学解析とその数値シミュレーションである。そのような有界領域内の粒子運動は、転位運動などの数理モデルにしばしば利用され、また SPH 法などの流体シミュレーション手法として重要である。しかし、領域境界における粒子運動の数学的に厳密な取り扱いの研究は多くなく、楊君の本研究はその数学的な基礎付けを与えるものとして価値の高いものである。博士論文は２つのパートからなり、前半は減衰効果が卓越した場合に相当する不連続項を含む１階の常微分方程式系に関するもので、様々な数値例とともに、弱い意味の解の定義を与え、吉田近似を用いてその一意性と大域可解性を証明している。これは同君の修士論文の発展で、SIAM J. Math. Anal., Vol.51 (2019) pp.5049-5076 として掲載済みである。後半は、ニュートンの運動法則で記述される２階の常微分方程式系に関するもので、境界での完全弾性衝突のため、加速度を測度として取り扱う必要が生じる。楊君はこの問題に対しても、弱解の定義を与え、大域可解性と条件付き一意性を示した（論文投稿中）。これらの結果には、新規性・独自性・有用性・発展性が認められる。以上により本論文は、博士(理学)を授与するに値すると判断した。

４．審査結果　(1) 判　　定（いずれかに○印）（合　格）・　不合格

(2) 授与学位　　博　士（　理 学　　）