

A Variational Formula for Conservation Laws Arising from Discrete Systems of Sticky Particles

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Abstract

In this paper, we study how discrete systems of sticky particles give rise to solutions of the conservation law $M_t + F(M)_x = 0$ for accumulated mass in one dimension. We show that the physically natural solution in the discrete setting is in fact the unique entropy solution to the conservation law. We then give a more detailed proof of a particle collision criterion of E, Rykov, and Sinai, and use this to verify a variational formula for the entropy solution which is a discretized version of the variational formula given in a pre-print of Tadmor and Wei.

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Introduction

In this paper, we study a mathematical model for finite systems of “sticky” particles in one dimension — particles that move along the x -axis with constant initial velocities until they collide, at which point they stick together, preserving mass and momentum. For motivation, we show how, if ρ is a smooth particle density obeying the laws of conservation of mass and momentum, then the accumulated mass function $M(x, t) = \int_{-\infty}^x \rho(s, t) ds$ for this system obeys its own conservation law, $M_t + F(M)_x = 0$ for a certain flux function F . We use this PDE as our starting point for the discussion of the discrete density case.

First we rigorously construct the physically intuitive model of the sticky particle system, working collision-by-collision and specifying the mass and velocity of each particle in the system at each time. This model in fact gives rise to a weak solution to the conservation law $M_t + F(M)_x = 0$ for piecewise-constant, non-decreasing, right-continuous initial data (i.e. initial data which are like the initial accumulated mass of a discrete particle system). Furthermore, we show that our weak solution obeys a condition on chord slopes on the graph of the flux function F , and is thus the unique entropy solution to the accumulated mass conservation law, by a result of Kruzhkov [3].

Having established a theoretical framework in which the sticky particle model is the natural solution to a partial differential equation, we then seek to give a more useful characterization of the state of the system at a given time. Since every other feature of the system (particle position, masses, and velocities) can be derived from the accumulated mass, this amounts to giving a clean characterization of $M(x, t)$ forward in time. For this, we discretize a closed-form variational formula for the smooth density system presented by Tadmor and Wei [5]. The key tool used in verifying the discrete variational formula is a collision criterion presented by E, Rykov, and Sinai [4], which allows

us to determine whether a group of particles has collided by checking a simple inequality involving only the initial positions, masses, and velocities of the particles involved. We give a thorough proof of a slight variation of this criterion, and use it to verify that the discrete variational formula describes our constructed sticky particle model.

1 The Smooth Density Model

1.1 Conservation Laws and Burgers' Equation

We begin with a smooth, non-negative function $\rho : \mathbb{R} \times [0, \infty) \rightarrow \mathbb{R}$. For each time $t \in [0, \infty)$, the function $\rho(\cdot, t)$ represents a fluid density in one dimension, and so the function $\rho(x, t)$ represents a smooth one-dimensional fluid density changing smoothly with time. We will also consider a smooth function $u : \mathbb{R} \times [0, \infty) \rightarrow \mathbb{R}$, which, at each fixed time t , gives a smooth vector field on \mathbb{R} which represents the flow velocity of the fluid. That is, the value $u(x, t)$ is the velocity of a particle at position x and time t . Such a system obeys a pair of partial differential equations called the *Euler equations*, which are

$$\rho_t + (\rho u)_x = 0 \tag{1.1a}$$

$$(\rho u)_t + (\rho u^2)_x = 0 \tag{1.1b}$$

and which we will derive from basic physical principles below.

First, for each starting position $x_0 \in \mathbb{R}$, we let $x(t, x_0)$ be the trajectory over time of a particle starting at x_0 according to the velocity field u . Formally, x solves the ordinary differential equation

$$\dot{x}(t, x_0) = u(x, t)$$

$$x(0, x_0) = x_0.$$

In order to derive the Euler equations for our fluid model, we assume formalizations of the principles of conservation of mass and momentum, respectively, and apply the *Reynolds transport theorem*. This theorem states (in one dimension) that if $\Omega(t) = (a(t), b(t))$ is a smoothly changing region in

\mathbb{R} and $f(x, t)$ is a smooth function, then

$$\frac{d}{dt} \int_{\Omega(t)} f(x, t) dx = \int_{\Omega(t)} f_t(x, t) dx + b'(t)f(b(t), t) - a'(t)f(a(t), t).$$

In order to apply this to the conservation of mass, we assume two things:

- (i) The region $\Omega(t)$ is a *closed system*; that is, that particles do not enter or leave $\Omega(t)$ over time.

Formally, $\Omega(t)$ moves according to the flow velocity:

$$\Omega(t) = x(\Omega_0, t).$$

- (ii) The mass of $\Omega(t)$ remains constant over time:

$$\int_{\Omega(t)} \rho(x, t) dx = \int_{\Omega_0} \rho(x, 0) dx.$$

We apply the transport theorem to this second criterion to deduce

$$0 = \frac{d}{dt} \int_{\Omega(t)} \rho(x, t) dx = \int_{\Omega(t)} \rho_t(x, t) dx + b'(t)\rho(b(t), t) - a'(t)\rho(a(t), t).$$

Note that, since the region moves according to the flow velocity, $a'(t) = u(a(t), t)$ and $b'(t) = u(b(t), t)$. Applying the divergence theorem (which, in the one-dimensional setting, is just the fundamental theorem of calculus),

$$0 = \int_{\Omega(t)} \rho_t + (\rho u)_x dx.$$

This allows us to deduce that $\rho_t + (\rho u)_x$ is in fact zero everywhere, by letting Ω be an arbitrary region and t a positive time, and applying the above calculation to the starting region $\Omega_0 = x(\Omega, -t)$ obtained by flowing Ω backwards for time t according to the flow velocity. Hence we have derived the *mass equation* (1.1a) from the principle of conservation of mass. An identical calculation, except requiring that *momentum* is conserved (according to Newton's second law, since we assume

no pressure or external forces are acting on the system):

$$\frac{d}{dt} \int_{\Omega(t)} \rho u \, dx = 0$$

gives the momentum equation (1.1b). Because of the types of physical interpretations we have just seen, PDEs of the form $u_t + F(u)_x$ are in general known as *conservation laws*.

If we assume that the density ρ is always positive, then subtracting u times the mass equation (1.1a) from the momentum equation (1.1b) and dividing through by ρ gives the *inviscid Burgers' equation* for the flow velocity:

$$u_t + uu_x = 0. \tag{1.2}$$

Also, Burgers' equation implies that

$$\frac{d}{dt} u(x(t, x_0), t) = u_x \dot{x} + u_t = u_t + uu_x = 0,$$

which means that the velocity field is constant along particle trajectories.

1.2 A Conservation Law for Accumulated Mass

We can calculate the accumulated mass of the density function:

$$M(x, t) = \int_{-\infty}^x \rho(x, t) \, dx,$$

and it turns out that M obeys a conservation law of the form $M_t + F(M)_x = 0$ as well. To see this, first note that

$$\begin{aligned} M_t &= \int_{-\infty}^x \rho_t \, dx \\ &= \int_{-\infty}^x (-(\rho u)_x) \, dx \\ &= -\rho u, \end{aligned}$$

using the mass equation and the fundamental theorem of calculus (Note this also requires an assumption $\lim_{x \rightarrow -\infty} \rho u = 0$, which we will assume). Also $M_x = \rho$, which implies that

$$M_t + uM_x = 0. \tag{1.3}$$

As with Burgers' equation above, this implies that $\dot{M}(x(t, x_0), t) = 0$ and thus that M is constant along particle trajectories, which matches physical intuition. Hence we can view the position of the particle starting at x_0 as a function $x_0(M)$ of the accumulated mass M . Furthermore, since u is constant along particle trajectories, i.e. $u(x(t, x_0), t) = u_0(x_0)$ for every t (from Burgers'), we can write

$$u(x(t, x_0), t) = u_0(x_0) = u_0(x_0(M)),$$

where M is the accumulated mass corresponding to the starting point x_0 , and thus we can write u as a function $u(x, t) = f(M(x, t)) = u_0(x_0(M(x, t)))$ of M . Letting F be an antiderivative of f , we thus have derived a conservation law for M :

$$M_t + F(M)_x = 0. \tag{1.4}$$

2 Discretization

2.1 Weak Solutions and the Jump Condition

We are interested in studying a discrete analogue of this problem: instead of a smooth particle density ρ , we would like to consider only a finite set of “sticky” (i.e. mass-and-momentum-preserving) particles. Naively, we would attempt to define a discrete density function, assigning a point mass and initial velocity to each particle starting position and proceed as in the smooth case. However, we immediately run into a problem, since in this model, not only are the density and velocity functions not differentiable — they are only non-zero at finitely many points. So we must adapt our above approach.

Instead, we will start from the conservation law for accumulated mass, equation (1.4). Formally,

we want M to be solution to the initial value problem

$$M_t + F(M)_x = 0 \quad (2.1a)$$

$$M(\cdot, 0) = M_0, \quad (2.1b)$$

where $M_0 : \mathbb{R} \rightarrow [0, \infty)$ is a right-continuous, piecewise-constant, finitely valued function, with $\lim_{x \downarrow -\infty} M_0(x) = 0$. Intuitively, M_0 is an initial accumulating mass function for a finite set of particles, each positioned at a point where M_0 has a jump.

Note that, in this model, the function M_0 is not continuous. Hence, we will not be able to find smooth solutions to (2.1), nor would we want to, since the discrete accumulated mass is naturally piecewise constant forward in time. So in order to “solve” (2.1), we use the concept of *weak* or *generalized* solutions to a conservation law:

Definition 2.1. *A bounded function $M : \mathbb{R} \times (0, \infty) \rightarrow [0, \infty)$ is called a weak solution to (2.1) if*

$$\int_0^\infty \int_{-\infty}^\infty M v_t + F(M) v_x \, dx \, dt + \int_{-\infty}^\infty M_0 v(\cdot, 0) \, dx = 0 \quad (2.2)$$

for every smooth, compactly supported, real-valued function $v(x, t)$ on $\mathbb{R} \times [0, \infty)$. In the case that M is smooth, this condition is equivalent to M being a solution of (2.1), which can be seen via integrating by parts (see [1] for more detail).

A well-known and important fact about weak solutions to conservation laws is the *Rankine-Hugoniot jump condition*, which is described in [1] as well: suppose that $(x(t), t)$ parameterizes a curve along which a weak solution $M(x, t)$ is discontinuous. Then

$$\frac{F(M^+) - F(M^-)}{M^+ - M^-} = \dot{x}, \quad (2.3)$$

where

$$M^+(x, t) = \lim_{y \downarrow x} M(y, t)$$

$$M^-(x, t) = \lim_{y \uparrow x} M(y, t)$$

are the left and right limits in space of M at time t .

2.2 Setting up the Discrete Model

From this starting point, we want to work backwards and recover density and velocity functions that agree with our intuitive understanding of the model and the relations that these quantities had with F in the smooth density model. Assume that $M(x, t)$ is a piecewise-constant weak solution to (2.1). Since we expect there to be a particle at each jump of M with mass equal to the height of the jump, we can define a “discrete density”

$$\rho(x, t) = M^+(x, t) - M^-(x, t).$$

We can then define the mass of a region Ω to be $\sum_{x \in \Omega} \rho(x, t)$, in analogy with the definition of mass for smooth ρ .

Slightly less transparently, we then define the flow velocity function by

$$u = \frac{F(M^+) - F(M^-)}{M^+ - M^-}, \tag{2.4}$$

letting it take on the value 0 if $M^+ = M^-$. The important thing to notice here is that, if M were a continuous function as in the smooth model, the limits involved in this equation would commute with the continuous function M , and result in the equality $u = F'(M)$, which was the defining property of F in the smooth model. Also, note that this definition of u agrees with the Rankine-Hugoniot condition (2.3), since we expect the velocity of the discontinuity of M to be the velocity of the particle causing the discontinuity.

Finally, some notation: We let x_1^0, \dots, x_n^0 denote the n points at which M_0 has jumps, and say the jump at x_i^0 has height m_i , i.e. $\rho(x_i, 0) = m_i$. Then the points x_i^0 represent the starting positions of the particles in the system, with m_i being the mass of the particle starting at x_i^0 (Figure 2.1). We will also refer to the “particle” x_i , which represents the propagating point mass of size m_i starting at position x_i^0 .

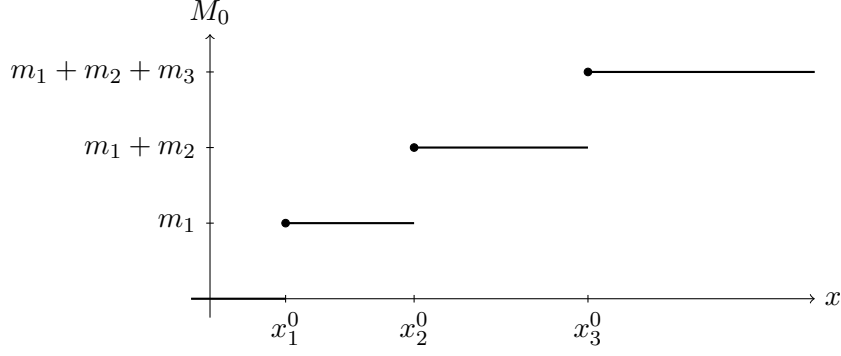


Figure 2.1: Initial accumulated mass for a three-particle system

2.3 Assumptions on F

First, we will illustrate by example that conditions must be imposed on F in order for the weak solution $M(x, t)$ to behave in a physically realistic manner. Suppose that we let F be an arbitrary smooth function, and consider the case where there is only one particle in the system, and it starts at position 0.

$$M_0(x) = \begin{cases} 0 & x < 0 \\ m & x \geq 0. \end{cases}$$

If we allow F to be smooth, and assume $F'(0) \leq F'(m)$, then the entropy solution to the PDE (2.1) is given in [1] by

$$M(x, t) = \begin{cases} 0 & \frac{x}{t} \leq F'(0) \\ (F')^{-1}\left(\frac{x}{t}\right) & F'(0) < \frac{x}{t} < F'(m) \\ m & \frac{x}{t} \geq F'(m) \end{cases}.$$

This is, of course, not physically realistic, since the mass function should be piecewise constant: for any fixed t , it should be zero before the current position of the single particle involved, and m afterward.

Closer consideration of F helps us determine a reasonable and effective condition to impose. Intuitively, $F'(M)$ is the velocity of the particle at which the accumulated mass is M . However, in this discrete system, the accumulated mass function only takes on finitely many values, so this interpretation does not quite make sense. Instead, we can interpret $F'(M)$ as the velocity of the

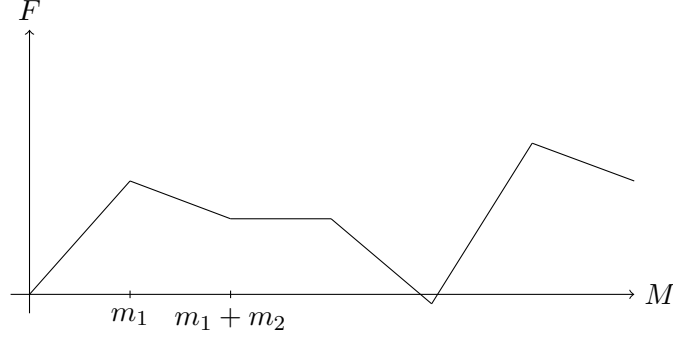


Figure 2.2: Piecewise affine flux function. The slope of the segment between $M = m_1$ and $M = m_1 + m_2$ is the initial velocity of x_2 .

rightmost particle at which the accumulated mass is bounded above by M . More formally, we can view $F'(M)$ as the velocity at the point at which the accumulated mass is equal to

$$\max_k \left\{ \sum_{i=1}^k m_i \leq M \right\}.$$

Hence it is reasonable to assume that F' is piecewise constant, with jumps occurring at the points $\sum_{i=1}^k m_i$ for $1 \leq k \leq n$. Note that F' is not necessarily nondecreasing. Of course, assuming that F' is piecewise constant is equivalent to assuming F is continuous and piecewise affine, so this is the condition that we will impose on F . Also note that the nodes of F occur at 0 and the points $\sum_{i=1}^k m_i$ for $1 \leq k \leq n$, and we interpret the slope of the chord connecting the two points

$$\left(\sum_{i=1}^{k-1} m_i, F \left(\sum_{i=1}^{k-1} m_i \right) \right) \quad \text{and} \quad \left(\sum_{i=1}^k m_i, F \left(\sum_{i=1}^k m_i \right) \right)$$

as the velocity of the particle starting at position x_k^0 . Formal justification of this will come a little later.

3 Solving the PDE

3.1 A Weak Solution

Consider the n -particle system:

$$M_0(x) = \begin{cases} 0 & x < x_1^0 \\ \sum_{k=1}^i m_k & x_i^0 \leq x < x_{i+1}^0, \quad i = 1, \dots, n-1 \\ \sum_{k=1}^n m_k & x_n^0 \leq x. \end{cases}$$

Letting $u_0 = u(\cdot, 0) = (F(M_0^+) - F(M_0^-))/(M_0^+ - M_0^-)$, this system has a weak solution

$$M(x, t) = \begin{cases} 0 & x < x_1(t) \\ \sum_{k=1}^i m_k & x_i(t) \leq x < x_{i+1}(t), \quad i = 1, \dots, n-1 \\ \sum_{k=1}^n m_k & x_n(t) \leq x, \end{cases}$$

where $x_i(t)$ is the trajectory of the particle x_i according to the initial velocity

$$v_i = u_0(x_i^0),$$

i.e. $x_i(t) = x_i^0 + tv_i$ (see [2]). Of course, this is only well-defined up until the point at which two of the trajectories $x_i(t)$, $x_j(t)$ intersect. We will extend the solution past these collision times using a shock wave.

Since the trajectories are continuous, the first collision must occur between some consecutive particle trajectories $x_k(t), \dots, x_{k+l}(t)$. That is, the first collision occurs when $x_k(t) = x_{k+1}(t) = \dots = x_{k+l}(t)$ for some $l > 0$. We continue the solution along a shock path: Let $t_{k,\dots,k+l}$ denote the time at which the trajectories intersect (note $t_{k,\dots,k+l} = (x_j^0 - x_i^0)/(v_i - v_j)$ for any $i, j \in \{k, \dots, k+l\}$). Then define a new trajectory

$$x_{k,\dots,k+l}(t) = x_k(t_{k,\dots,k+l}) + u(x_k(t_{k,\dots,k+l}), t_{k,\dots,k+l})(t - t_{k,\dots,k+l}),$$

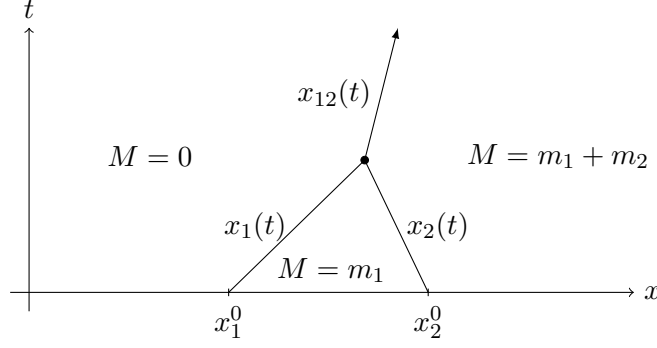


Figure 3.1: A two-particle collision.

(where u is defined as in (2.4)) and, for $t \geq t_{k,\dots,k+l}$ and x near this new particle trajectory, define

$$M(x, t) = \begin{cases} \sum_{i=1}^{k-1} m_i & x < x_{k,\dots,k+l}(t), \\ \sum_{i=1}^{k+l} m_i & x_{k,\dots,k+l}(t) \leq x. \end{cases}$$

This defines a weak solution of the conservation law (2.1) for all $t > 0$ (see [2]).

For notational clarity, we will use a multi-index notation for collisions: If $\alpha = \{k, \dots, k+l\}$ is a set of consecutive indices, and if the particles x_i for $i \in \alpha$ collide, we will say they collide at time t_α to form a new particle x_α moving along the trajectory $x_\alpha(t)$ for $t \geq t_\alpha$. Also, for two consecutive sets of indices α and β , we will denote their union by $\alpha\beta$. This will be used, for instance, in the collision of two clusters x_α and x_β to form a new cluster $x_{\alpha\beta}$.

3.2 Conservation of Mass and Momentum

Now we will argue that this solution preserves mass and momentum. First, mass is preserved along particle trajectories away from collisions, since $\rho(x, t)$ is just a propagating constant point mass along such a trajectory. And since a collision replaces a set of particles with masses m_k, \dots, m_{k+l} with a single point mass of size $m_k + \dots + m_{k+l}$, mass is conserved through collisions as well.

A bit more analysis is required to show that momentum is conserved. We will prove that momentum is conserved through a single collision of two particle clusters; the argument for an l -particle collision is the same, and we can get the full result (after multiple collisions) by induction. So consider two adjacent clusters x_α and x_β . By construction, these trajectories have velocities $u(x_\alpha(t_\alpha), t_\alpha)$ and $u(x_\beta(t_\beta), t_\beta)$ respectively. And since $u := (F(M^+) - F(M^-))/(M^+ - M^-)$, we

have that

$$\begin{aligned} u(x_\alpha(t_\alpha), t_\alpha) &= \frac{F(M_{k+l}) - F(M_{k-1})}{M_{k+l} - M_{k-1}} \\ u(x_\beta(t_\beta), t_\beta) &= \frac{F(M_{k+p}) - F(M_{k+l})}{M_{k+p} - M_{k+l}}, \end{aligned}$$

where here we let M_j denote $\sum_{i=1}^j m_i$, for notational ease. Since the particle cluster x_α has mass $m_k + \dots + m_{k+l} = M_{k+l} - M_{k-1}$ and the second has mass $m_{k+l+1} + \dots + m_{k+p} = M_{k+p} - M_{k+l}$, the pre-collision momentum of these two particle clusters is

$$\begin{aligned} &(m_k + \dots + m_{k+l}) \frac{F(M_{k+l}) - F(M_{k-1})}{M_{k+l} - M_{k-1}} + (m_{k+l+1} + \dots + m_{k+p}) \frac{F(M_{k+p}) - F(M_{k+l})}{M_{k+p} - M_{k+l}} \\ &= F(M_{k+p}) - F(M_{k-1}). \end{aligned}$$

Similarly, the post-collision cluster has velocity

$$\frac{F(M_{k+p}) - F(M_{k-1})}{M_{k+p} - M_{k-1}},$$

and mass $m_k + \dots + m_{k+p} = M_{k+p} - M_{k-1}$, and thus its momentum is equal to the combined pre-collision momenta of the two particles. Hence momentum is conserved through collisions.

An importance consequence of the conservation of momentum is the following: if n particles x_1, \dots, x_n have collided by time t , then the momentum of the post-collision cluster is

$$\sum_{i=1}^n m_i v_i,$$

and thus the cluster has velocity

$$\frac{\sum_{i=1}^n m_i v_i}{\sum_{i=1}^n m_i}.$$

4 Uniqueness of the Weak Solution

In addition to the fact that our constructed solution obeys the physical laws of conservation of mass and momentum, there is a more formal sense in which it is the most “natural” solution to (2.1). In [3], Kruzhkov defines a technical condition that can be imposed on weak solutions to conservation laws of the form $M_t + F(M)_x = 0$. The details of the general Kruzhkov condition are beyond the scope of this paper, but we state the condition here for completeness: A weak solution M to the conservation law (2.1) is an *entropy solution* if

$$\int_0^\infty \int_{-\infty}^\infty \operatorname{sgn}(M - k) \phi_t + (F(M) - F(k)) \phi_x \, dx \, dt \geq 0$$

for every C^1 , compactly supported, non-negative test function $\phi : \mathbb{R} \times [0, \infty) \rightarrow \mathbb{R}$ and every $k \in \mathbb{R}$.

In [2], Bressan shows that, in the case of bounded, piecewise-constant initial data, a weak solution is an entropy solution if and only if both the Rankine-Hugoniot conditions (2.3) and the following condition hold:

Definition 4.1. *A weak solution M obeys the chord condition if, at any discontinuity of $M(x, t)$,*

$$\frac{F(M) - F(M^-)}{M - M^-} \geq \frac{F(M^+) - F(M^-)}{M^+ - M^-} \geq \frac{F(M^+) - F(M)}{M^+ - M}, \quad (4.1)$$

for all $M \in (M^-, M^+)$.

Geometrically, this condition says that whenever $M(\cdot, t)$ has a discontinuity (i.e. $M^- < M^+$), the chord connecting the points $(M^-, F(M^-))$ and $(M^+, F(M^+))$ in the FM -plane does not cross the graph of the flux function F . Note that since we allow equality, the chord may coincide with the graph of F as long as it does not cross from one side to the other.

Kruzhkov proves in [3] that there is at most one bounded entropy solution to (2.1). Since our construction $M(x, t)$ obeys the Rankine-Hugoniot condition as seen in section 2.2, the following theorem establishes that our construction is the unique bounded entropy solution to (2.1):

Theorem 4.1. *Our constructed solution $M(x, t)$ obeys the chord condition (4.1), and is thus the unique bounded entropy solution to (2.1).*

Proof. It is easy to see that the chord condition holds for M before any collisions occur: before any

collisions, F is a piecewise affine function with nodes at exactly the discontinuities $M_k := \sum_{i=1}^k m_i$ for $k = 1, \dots, n$ of M . Hence the chords coincide exactly with the graph of F , and we have equality in (4.1) for all $M \in (M^-, M^+)$.

In order to demonstrate that the chord condition continues to hold after finitely many collisions, we introduce the idea of a flux function that changes after each collision. For notational simplicity, assume that the first collision occurs between two consecutive particles x_k and x_{k+1} , at time $t = t_{k,k+1}$. Then for $t \geq t_{k,k+1}$, the function $M(x, t)$ is a weak solution to the problem

$$\begin{aligned} M_t + F^1(M)_x &= 0 \\ M(\cdot, t_{k,k+1}) &= M^1, \end{aligned}$$

where M^1 has a jump of height m_i at $x_i(t_{k,k+1})$ for $i \neq k, k+1$ and a jump of height $m_k + m_{k+1}$ at $x_k(t_{k,k+1}) = x_{k+1}(t_{k,k+1})$ (that is, the particles with mass m_k and m_{k+1} at positions $s_k(t)$ and $s_{k+1}(t)$ have been replaced by a particle of mass $m_k + m_{k+1}$ at their mutual current location). And $F^1(M)$ agrees with F except on $[M_k, M_{k+1}]$, where we have

$$F^1(M) = F(M_k) + \frac{F(M_{k+1}) - F(M_k)}{M_{k+1} - M_k}(M - M_k).$$

That is, on $[M_k, M_{k+1}]$, the graph of F has been replaced by the chord connecting $(M_k, F(M_k))$ and $(M_{k+1}, F(M_{k+1}))$. Proceeding inductively, we obtain a new flux function after each collision, and since the discontinuities of M at some time t are exactly the nodes of the flux function corresponding to the state of the system at that time, we can say that M obeys the chord condition if and only if the graph of the evolving flux function never crosses the graph of the original flux function F .

And we can prove inductively that it never crosses: suppose that the system undergoes some finite number K of collisions, with corresponding flux functions $F = F^0, F^1, F^2, \dots, F^K$. We've seen that the chord condition holds before the first collision, which we can now phrase as the statement that the graph of F does not cross itself. Now assume that the chord condition still holds after the K -th collision; that is, that the graph of F^K does not cross the graph of F . We must argue that the graph of F^{K+1} also does not cross the graph of F . To see this, say that the K -th collision occurred at time t_K , and that the $(K+1)$ -st collision will occur between r consecutive

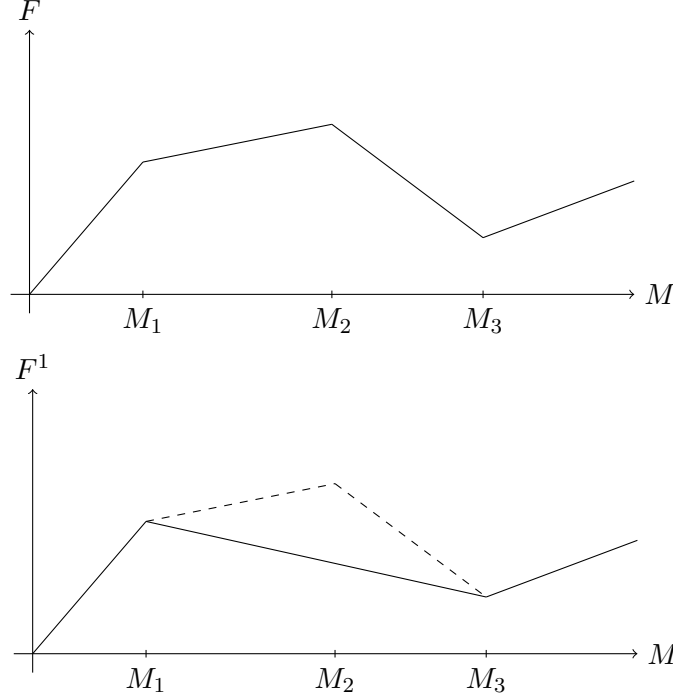


Figure 4.1: Initial evolution of the flux function if particles x_2 and x_3 collide first.

clusters $x_{\alpha_1} < \dots < x_{\alpha_r}$, with trajectories $x_{\alpha_i}(t) = x_{\alpha_i}(t_K) + u(x_{\alpha_i}(t_K), t_K)(t - t_K)$ for $1 \leq i \leq r$ and $t \geq t_K$, and masses m_{α_i} . Then collision at time t_{k+1} implies that

$$u(x_{\alpha_i}(t_K), t_K) - u(x_{\alpha_{i+1}}(t_K), t_K) = \frac{x_{\alpha_{i+1}}(t_K) - x_{\alpha_i}(t_K)}{t_{K+1} - t_K} > 0,$$

or, simply that the velocity of each particle involved in the collision is greater than the velocity of the particle to its immediate right. But recall that the velocity is given by $u = (F^K(M^+) - F^K(M^-))/(M^+ - M^-)$; that is, the velocity u of a particle is the chord slope of the affine segment of the flux function over the mass jump corresponding to that particle. In particular,

$$u(x_{\alpha_i}(t_K), t_K) = \frac{F^K(M_{\alpha_i}) - F^K(M_{\alpha_{i-1}})}{M_{\alpha_i} - \hat{M}_{\alpha_{i-1}}}.$$

where the points $M_{\alpha_i} = \sum_{j=1}^i m_{\alpha_j}$ are exactly the nodes of the flux function F^K . This means that F^K is affine on each interval $[M_{\alpha_i}, M_{\alpha_{i+1}}]$, and that the slope of F^K on $[M_{\alpha_i}, M_{\alpha_{i+1}}]$ is strictly smaller than the slope on $[M_{\alpha_{i+1}}, M_{\alpha_{i+2}}]$. Hence, F^K is a concave function on $[M_{\alpha_1}, M_{\alpha_r}]$ and in particular, the chord connecting $(M_{\alpha_1}, F^K(M_{\alpha_1}))$ and $(M_{\alpha_r}, F^K(M_{\alpha_r}))$ lies below the graph of F^K .

Now, we are ready to show that the chord condition holds post-collision. Observe that the post- K -th-collision flux function F^{K+1} is equal to F^K except on $[M_{\alpha_1}, M_{\alpha_r}]$, where its graph has been replaced by the chord between $(M_{\alpha_1}, F^K(M_{\alpha_1}))$ and $(M_{\alpha_r}, F^K(M_{\alpha_r}))$. As we just argued, this chord lies below the graph of F^K . Applying induction, we can conclude that this chord also lies below the graph of the original flux function $F^0 = F$, which proves that M satisfies the chord condition even after collisions.

□

5 The ERS Collision Criterion

Now that we have shown that the “sticky particle” model is the unique solution to the accumulated mass conservation law, we look for a simpler characterization of the solution $M(x, t)$. In this section, we will give a more detailed proof of the following collision criterion, a slight modification of which is presented and proved by E, Rykov, and Sinai in [4]. This criterion will be the key tool used to verify the variational formula for computing $M(x, t)$ in the next section.

Theorem 5.1. *Let $x_1^0 < x_2^0 < \dots < x_n^0$ be the initial positions of n particles x_1, \dots, x_n , and suppose that these particles do not interact with any other particles before time t . Then x_1, \dots, x_n will have collided to form a single particle cluster by time t if and only if*

$$\frac{\sum_{i=1}^k m_i(x_i^0 + u_0(x_i^0)t)}{\sum_{i=1}^k m_i} \geq \frac{\sum_{i=1}^n m_i(x_i^0 + u_0(x_i^0)t)}{\sum_{i=1}^n m_i} \quad (5.1)$$

for all $k \in \{1, \dots, n\}$.

Note that this condition, which we will call ERS, says that we can determine whether or not a group of particles has collided by only looking at their *initial* (before any collisions have occurred) trajectories. Also observe that the left-hand side of this inequality is the propagating center of mass of the initial trajectories of the k left-most particles, and the right-hand side is the analogous quantity for the entire collection of particles.

In order to prove this theorem, we will introduce some new notation and several lemmas. First,

for a set of consecutive indices $\alpha = \{k, \dots, k+l\}$ in $\{1, \dots, n\}$, we define

$$X_\alpha(t) = \frac{\sum_{i \in \alpha} m_i(x_i^0 + tv_i)}{\sum_{i \in \alpha} m_i} = \frac{\sum_{i=k}^{k+l} m_i(x_i^0 + tv_i)}{\sum_{i=k}^{k+l} m_i},$$

where $v_i = u_0(x_i^0)$ is the initial velocity of particle x_i . That is, $t \mapsto X_\alpha(t)$ is the propagating center of mass of the *original* trajectories of the particles with indices in α . Now we present three lemmas:

Lemma 5.1. *Suppose that particles x_i for $i \in \alpha$ have collided to form a single cluster x_α by time t^* . Then for $t > t^*$, as long as no other particles have collided with x_α , the path of the cluster is given by $X_\alpha(t)$.*

Proof. We wish to prove that the post-collision trajectory coincides with the center of mass of the initial particle trajectories past the collision time. To prove this, note that we have proved conservation of momentum for the particle systems, which means that the post-collision cluster has velocity

$$\frac{\sum_{i \in \alpha} m_i v_i}{\sum_{i \in \alpha} m_i} = \frac{d}{dt} X_\alpha(t).$$

So the two trajectories in question are lines with the same slope. So in order to prove our proposition, we must show that they agree at a point. We will show by induction that they agree at collision time. Formally, we will show by induction that two particle clusters x_α and x_β colliding at $t = t_{\alpha\beta}$ will be at position $X_{\alpha\beta}(t_{\alpha\beta})$ at collision time. For notational ease, we will reason through two collisions, and how to proceed inductively will be clear. Consider three particles x_1, x_2, x_3 . Say x_1 and x_2 collide first. Then when they collide, their positions are the same, so their center of mass $X_{12}(t_{12})$ is located at their mutual location, which is the starting point of the post-collision trajectory. Hence the claim holds after a single collision. Next, when x_{12} and x_3 collide, their center of mass will be at their mutual location $x_{12}(t_{123}) = x_3(t_{123}) = X_{12}(t) = X_3(t)$. That is, their location is the center of mass of the following two quantities: the center of mass of $x_1^0 + t_{123}v_1$ and $x_2^0 + t_{123}v_2$, and $x_3^0 + t_{123}v_3$. But since taking center of mass is an associative operation, this location is the center of mass of all three $x_i + t_{123}v_i$ for $i = 1, 2, 3$, or in other words, $X_{123}(t_{123})$. Hence the center of mass of the three initial trajectories passes through the collision point. This lets us conclude that $X_{123}(t)$ and the path of x_{123} are the same line, and induction proves the lemma. \square

Lemma 5.2. *Suppose that $x_\alpha < x_\beta$ are two consecutive particle clusters that collide at time $t_{\alpha\beta}$.*

Then for $t > t_{\alpha\beta}$ we have

$$X_\beta(t) < X_{\alpha\beta}(t) < X_\alpha(t).$$

Proof. For $t < t_{\alpha\beta}$, the trajectories of x_α and x_β are given by $X_\alpha(t)$ and $X_\beta(t)$, respectively, by Lemma 5.1. Since the two particles have not collided before $t_{\alpha\beta}$ and their paths are affine functions of t , we have

$$X_\alpha(t) < X_\beta(t), \quad t < t_{\alpha\beta}$$

$$X_\alpha(t) = X_\beta(t), \quad t = t_{\alpha\beta}$$

$$X_\alpha(t) > X_\beta(t), \quad t > t_{\alpha\beta}.$$

In particular, we have $X_\beta(t) < X_\alpha(t)$ post-collision. Now note that $X_{\alpha\beta}(t)$ is a *convex combination* of $X_\beta(t)$ and $X_\alpha(t)$, since

$$\begin{aligned} X_{\alpha\beta}(t) &= \frac{\sum_{i \in \alpha} m_i}{\sum_{i \in \alpha} m_i + \sum_{j \in \beta} m_j} \frac{\sum_{i \in \alpha} m_i (x_i^0 + tv_i)}{\sum_{i \in \alpha} m_i} + \frac{\sum_{j \in \beta} m_j}{\sum_{i \in \alpha} m_i + \sum_{j \in \beta} m_j} \frac{\sum_{j \in \beta} m_j (x_j^0 + tv_j)}{\sum_{j \in \beta} m_j} \\ &= \delta X_\alpha(t) + (1 - \delta) X_\beta(t), \end{aligned}$$

where $\delta = \frac{\sum_{i \in \alpha} m_i}{\sum_{i \in \alpha} m_i + \sum_{j \in \beta} m_j} \in (0, 1)$. Hence we can conclude that $X_{\alpha\beta}(t)$ lies strictly between $X_\beta(t)$ and $X_\alpha(t)$ post-collision:

$$X_\beta(t) < X_{\alpha\beta}(t) < X_\alpha(t)$$

for $t > t_{\alpha\beta}$, which is exactly what we wanted to prove. \square

Lemma 5.3. *Suppose that $x_1, \dots, x_k, x_{k+1}, \dots, x_{k+l}$ are consecutive particles, and that x_{k+1}, \dots, x_{k+l} have collided to form a cluster x_β (subsets of x_1, \dots, x_k may or may not have already collided). Assume that x_β collides with (the cluster containing) x_k at some time t^* . Then, letting $\alpha = \{1, \dots, k\}$,*

$$X_{\alpha\beta}(t) < X_\alpha(t)$$

for $t > t^$. In other words: if a cluster enters a group of particles from the right, then the center of mass of the entire group is moved to the left.*

Proof. Suppose that the particles x_1, \dots, x_k have collided to form clusters $x_{\alpha_1}, \dots, x_{\alpha_K}$ leading up to the collision time of $\{x_1, \dots, x_k\}$ with x_β . By Lemma 5.2, we know that

$$X_\beta(t) < X_{\alpha_K\beta}(t) < X_{\alpha_K}(t)$$

for $t > t^*$. In particular, $X_{\alpha_K\beta}(t) < X_{\alpha_K}(t)$. And since all cluster locations $X_{\alpha_1}(t), \dots, X_{\alpha_{K-1}}(t)$ lie strictly to the left of both $X_{\alpha_K\beta}(t)$ and $X_{\alpha_K}(t)$, we know that the center of mass of $X_{\alpha_1}(t), \dots, X_{\alpha_K}(t)$ must be strictly less than the center of mass of $X_{\alpha_1}(t), \dots, X_{\alpha_K}(t), X_\beta(t)$ (using both the fact that collisions within $x_{\alpha_1}, \dots, x_{\alpha_K}$ will not affect their center of mass, and the assumption that no particles collide with these clusters from the left). But by associativity of center of mass, this simply means that $X_\alpha(t) < X_{\alpha\beta}(t)$ for $t > t^*$, which is what we wanted to show \square

Now we are ready to present the proof of the collision criterion, Theorem 5.1:

Proof. One direction is straightforward: Suppose that the particles x_1, \dots, x_n have not all collided to form a single cluster by time t . In particular, suppose that they have formed clusters $x_{\alpha_1}, \dots, x_{\alpha_K}$. Then for any $J \in \{1, \dots, K-1\}$ we have that the center of mass of $x_{\alpha_1}, \dots, x_{\alpha_J}$ lies strictly to the left of that of $x_{\alpha_{J+1}}, \dots, x_{\alpha_K}$. By associativity, this implies $X_{\alpha_1 \dots \alpha_J}(t) < X_{\alpha_1 \dots \alpha_K}(t)$, which means that the ERS criterion fails at $k = \max \alpha_J$.

For the second direction, we make use of Lemmas 5.1 through 5.3. Assume that the particles x_1, \dots, x_n have all collided by time t , but that the condition 5.1 fails for some k . This means that $X_{\{1, \dots, k\}}(t) < X_{\{1, \dots, n\}}(t)$. However, this contradicts Lemma 5.3: Since we assumed that no other particles interact with x_1, \dots, x_n , the set of particles x_1, \dots, x_n is formed as clusters of particles hit $\{x_1, \dots, x_k\}$ from the right, one at a time. Hence, using induction and Lemma 5.3 implies that $X_{\{1, \dots, n\}}(t) < X_{\{1, \dots, k\}}(t)$. This is a contradiction, which completes the proof. \square

6 Variational Formula

Tadmor and Wei [5] provide the following variational formula for solutions of the mass and momentum equations in the smooth case:

$$M(x, t) = \int_{-\infty}^{y(x, t)} \rho_0(s) ds,$$

where $y(x, t)$ is defined as

$$y(x, t) = \sup \left\{ \operatorname{arginf}_y \int_{-\infty}^y (s + tu_0(s) - x) \rho_0(s) ds \right\}.$$

Since our sticky particle system is a solution to a discretization of the mass and momentum equations, we would expect it to satisfy a discretized version of the variational formula, and it in fact does:

Theorem 6.1. *The unique entropy solution to the sticky particle problem (2.1) is given by the formula*

$$M(x, t) = \sum_{i | x_i^0 < y(x, t)} m_i,$$

where

$$y(x, t) = \sup \left\{ \operatorname{arginf}_y \sum_{i | x_i^0 \leq y} m_i(x_i^0 + tv_i - x) \right\}.$$

For fixed x and t , we will denote the functional $\sum_{i | x_i^0 \leq y} m_i(X_i(t) - x)$ by $S(y)$, and note that $x_i^0 + tv_i = X_i(t)$. Now, to begin proving 6.1, first note that $y(x, t)$ must have the form x_k^0 for some k , since $S(y) = S(\hat{y})$ for all $\hat{y} \in [y, x_0^k)$, where x_0^k is the smallest particle starting position to the right of y . Hence minimizing $S(y)$ over y amounts to minimizing $S_k := \sum_{i=1}^k m_i(X_i(t) - x)$ over k . Also, basic algebraic manipulation with centers of mass tells us that if the particle x_j belongs to the cluster x_{α_J} , then

$$\sum_{i=1}^j m_i(X_i(t) - x) = \sum_{I=1}^{J-1} m_{\alpha_I}(X_{\alpha_I}(t) - x) + \sum_{\substack{i \leq j \\ i \in \alpha_J}} m_i(X_i(t) - x), \quad (6.1)$$

where $m_{\alpha_I} = \sum_{i \in \alpha_I} m_i$.

Now, we state a lemma which is trivial to prove but which we include for the sake of clarity of the argument:

Lemma 6.1. *If $x_\alpha(t) \leq x$ (i.e. x_α is a cluster which lies to the left of position x at time t), then $m_\alpha(X_\alpha(t) - x) \leq 0$; and if $x_\alpha(t) > x$, then $m_\alpha(X_\alpha(t) - x) > 0$. In other words, clusters lying to the left of x have net non-positive contributions to the sum $\sum m_\alpha(X_\alpha(t) - x)$, and clusters lying (strictly) to the right have net positive contributions.*

Next, we prove a lemma making use of the collision criterion 5.1 from the previous section:

Lemma 6.2. *Let j be an index, with x_j belonging to the cluster x_α . Then*

$$\sum_{\substack{i \leq j \\ i \in \alpha}} m_i(X_i(t) - x) \geq m_\alpha(X_\alpha(t) - x) \quad \text{if } x_\alpha(t) \leq x$$

and

$$\sum_{\substack{i \leq j \\ x \in \alpha}} m_i(X_i(t) - x) > 0 \quad \text{if } x_\alpha(t) > x.$$

In other words, left partial clusters of clusters lying to the left of x do not contribute more negatively than the total cluster, and left partial clusters of clusters lying to the right of x contribute positively.

Proof. For the first part, assume for contradiction that

$$\sum_{\substack{i \leq j \\ i \in \alpha}} m_i(X_i(t) - x) < m_\alpha(X_\alpha(t) - x) \leq 0.$$

Since $0 < \sum_{\substack{i \leq j \\ i \in \alpha}} m_i < m_\alpha$, we can divide and preserve the inequality:

$$\frac{\sum_{\substack{i \leq j \\ i \in \alpha}} m_i(X_i(t) - x)}{\sum_{\substack{i \leq j \\ i \in \alpha}} m_i} < X_\alpha(t),$$

which contradicts Theorem 5.1.

For the second part, simply note that by Theorem 5.1,

$$\sum_{\substack{i \leq j \\ i \in \alpha}} m_i(X_i(t) - x) \geq X_\alpha(t) > x,$$

which, subtracting x from each quantity, yields

$$\frac{\sum_{\substack{i \leq j \\ i \in \alpha}} m_i (X_i(t) - x)}{\sum_{\substack{i \leq j \\ i \in \alpha}} m_i} \geq X_\alpha(t) - x > 0,$$

which gives the desired result. □

Now we can prove Theorem 6.1:

Proof. Let $k = \max \alpha_K$, where K is the index for which $x \in [x_{\alpha_K}, x_{\alpha_{K+1}})$, at time t , and we claim that the largest index at which the sum $\sum_{i=1}^j m_i (X_i(t) - x)$ is minimized is at $j = k$. Since we take the supremum of all minimizers, this will imply that $y(x, t) = \min \alpha_{K+1}$ is the initial position of the leftmost particle composing the first cluster that lies strictly to the right of x . Note that this claim implies the desired result, since $\sum_{i|X_i(t) < x} m_i$ will be the total mass of all of the clusters to the left of x at time t , which is precisely the accumulated mass at (x, t) for the entropy solution.

This claim is immediate from the combination of the previous two lemmas: The first lemma says that terms of the form $m_{\alpha_I} (X_{\alpha_I}(t) - x)$ for $I \leq K$ contribute non-positively to the sum as written in (6.1), and the second lemma says that the minimum cannot occur inside such a cluster. In other words, $\sum_{i=1}^j m_i (X_i(t) - x)$ is a non-decreasing function of j for $j \leq \max \alpha_K$. Hence, $S(y)$ is minimized at $y = x_0^k$. Similarly, the first and second lemmas combine to say that all terms after $j = k$ contribute positively to the sum, so the fact that $y(x, t)$ is the *supremum* of all minimizers of $S(y)$ allows us to conclude that it is in fact the case that $y(x, t) = x_0^k$, and thus that the variational formula gives $M(x, t) = m_1 + \cdots + m_k$, which is the total mass to the left of x at time t as desired. □

Conclusions and Future Work

In summary, we have situated the sticky particle problem within a theoretical framework as the unique entropy solution to a conservation law, and have ultimately given a compact variational formula for the accumulated mass function of the system at any positive time. Along the way, we also proved the extremely useful ERS particle collision criterion.

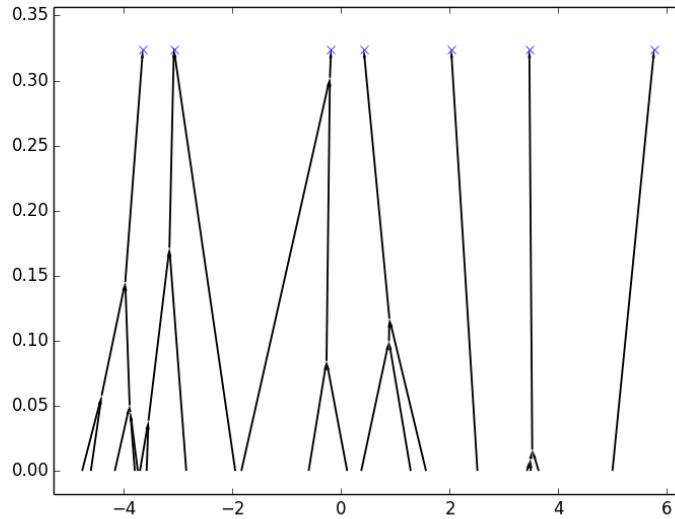


Figure 6.1: A simulation of collisions in a 20-particle system.

Even without going beyond the scope of this paper, it is easy to see why these results are useful: they make it much easier to model sticky particle systems computationally. For instance, we used the ERS criterion to write a simple Python program which displays the particle cluster paths forward in time, and used the variational formula to create an animation of the evolution of the accumulated mass function, in just a few lines of code — neither of these would have been feasible using only our initial collision-by-collision characterization of the system (see Figure 6.1).

But the results become even more useful if we can use them to understand broader classes of particle systems. In particular, can we use discrete particle models to approximate smooth-density systems? In order to answer this question, we need to understand how perturbations in initial data affect the accumulated mass in discrete systems. More precisely, the metric $d(M, \hat{M}) = \|M^{-1} - \hat{M}^{-1}\|_\infty$ is a natural way to measure distance between accumulated mass functions. If \hat{x}_i^0, \hat{v}_i are initial data for a perturbed system, can we bound $d(M, \hat{M})$ given bounds, say $|x_i^0 - \hat{x}_i^0| < \epsilon_x$, $|v_i - \hat{v}_i| < \epsilon_v$, on the perturbations? Clearly $|x_i(t) - \hat{x}_i(t)| < \epsilon_x + \epsilon_v t$ before any collisions, but what happens if different particles end up in different clusters in the perturbed system? Can we use ERS to bound the distances between the clusters in the perturbed systems and clusters that share an initial point from the original system? See [6] for details.

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