

Toy Model of Shock Flow

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Received April 2, 2022

Abstract. We consider one-dimensional flow of point particles towards the wall. The only interaction between neighboring particles are elastic collisions. We consider the limiting transition to continuum mechanics, when number of particles tends to infinity and the distance between neighboring particles tends to zero. We show that, as a result of the shock, the sharp break appears between regions with initial and double initial densities.

KEYWORDS: micro-macro continuum mechanics, shock flow, cellular automata, point particles, collisions

AMS SUBJECT CLASSIFICATION: 70F45

1. Introduction

One of the important problems in mathematical physics is to deduce the macro laws of continuum mechanics from micro laws of point particles mechanics. However, the attempts to do this were only with strongly stochastic micro dynamics. Purely deterministic way was suggested in fact in the following two papers:

1. In [2], where simple models without interaction but with external forces were considered. The notion of regularity (no intersection of particle trajectories) were introduced.

2. In [1] where systems of N particles with mutual interaction were considered, moreover, distances between neighboring particles were of the order $\frac{1}{N}$ but not less than $\frac{\varepsilon}{N}$ with $0 < \varepsilon$ not dependent on N . Euler equation, which was obtained in this paper, appeared (very unexpectedly for us) to coincide with the known Euler equation for one-dimensional Chaplygin gas, see [5, 6].

Here we consider simplest model with collisions but without external forces and where collision is the only possible interaction between particles. Note that collision models cannot be regular by definition (see [2]).

Already here there are interesting phenomena in continuum limit. We will immediately see two kinds of continuum limits for micro dynamics. This is due to the absence of smoothness in the dynamics. This shows that the relation between micro models in particle mechanics and macro models in continuum mechanics may be more complicated than just a transition from many particle ordinary differential equations to partial differential equations.

2. Model and Results

In general, at any time $0 \leq t < \infty$ we have N identical (equal masses) point particles $1, 2, \dots, N$ on R_+ with initial coordinates

$$0 < x_1(0) < \dots < x_N(0) \quad (2.1)$$

and negative initial velocities

$$v_1(0) < 0, \dots, v_N(0) < 0 \quad (2.2)$$

There are no any external forces and interaction (except collisions) between particles. When particle 1 collides with the wall (the point $x_0 = 0$), its velocity changes the sign. When two particles collide they exchange velocities. We agree that always at the moments t of collisions $v_k(t)$ of any particle k means $v_k(t+0)$.

Remark 1. Collisions with external force for 2 particle system were considered in [3] (see also [4]), where relation of such model with billiard dynamical systems and with number π was discovered.

Below we consider the simplest cases, related by scaling $x \rightarrow \frac{x}{N}, t \rightarrow \frac{t}{N}$. Namely, for $k = 1, 2, \dots, N$

$$x_k(0) = k, \quad v_k(0) = -1 \quad (2.3)$$

and

$$x_k(0) = \frac{k}{N}, \quad v_k(0) = -1, \quad (2.4)$$

together with the limit $N \rightarrow \infty$ to get continuum mechanics model.

2.1. Continuum limit

Density. Now we consider the case (2.4) of initial conditions. Define distribution function (of the number of particles) at time t as

$$F_N(x, t) = \frac{1}{N} \#\{k : x_k(t) < x\}, \quad 0 < x < \infty$$

It is clear that at time 0 there exists, as $N \rightarrow \infty$, continuum limit of the distribution function

$$F(x, 0) = \lim_{N \rightarrow \infty} F_N(x, 0) = x, \quad 0 < x < 1,$$

and the density

$$\rho(x, 0) = F_x(x, 0) = 1, \quad 0 < x < 1.$$

Theorem 1. For any time $t \geq 0$ there exists the limit

$$F(x, t) = \lim_{N \rightarrow \infty} F_N(x, t),$$

and the function (density) $\rho(x, t)$ such that

$$\int_0^x \rho(x, t) dx = F(x, t)$$

Moreover, for $0 < t < \frac{1}{2}$

$$\rho(x, t) = \begin{cases} 2, & 0 < x < t \\ 1, & t < x < 1 - t \\ 0, & 1 - t < x < \infty, \end{cases}$$

for $\frac{1}{2} \leq t < 1$

$$\rho(x, t) = \begin{cases} 2, & 0 < x < 1 - t \\ 1, & 1 - t < x < t \\ 0, & t < x < \infty, \end{cases}$$

and for $t \geq 1$

$$\rho(x, t) = \begin{cases} 0, & 0 < x < t - 1, \\ 1, & t - 1 < x < t, \\ 0 & t < x. \end{cases}$$

Lagrangian trajectories. For any $x \in [0, 1]$ and any N we define particle (index) $k = k(N, x)$ such that its initial coordinate $x_k(0) = x_{k(N, x)}(0)$ is the closest from x (say, from the right). Let $x_k(t) = x_{k(N, x)}(t)$ be the trajectory of this particle.

We call (if this limit exists)

$$y(x, t) = \lim_{N \rightarrow \infty} x_{k(N, x)}(t) \tag{2.5}$$

the Lagrangian trajectory of the continuum media “particle” which is initially at point x .

Theorem 2. *The limit (2.5)*

$$y(x, t) = \lim_{N \rightarrow \infty} x_{k(N,x)}(t)$$

exists for any $t \geq 0$ and is equal to

$$y(1, t) = \begin{cases} 1 - t, & t \leq \frac{1}{2}, \\ t, & t > \frac{1}{2}, \end{cases} \quad y(0, t) = \begin{cases} 0, & t \leq 1, \\ t - 1, & t > 1, \end{cases}$$

$$y(x, t) = \begin{cases} x - t, & t < \frac{x}{2}, \\ \frac{x}{2}, & \frac{x}{2} \leq t < \frac{1}{2}, \\ \frac{x}{2} + (t - \frac{1}{2}), & t \geq \frac{1}{2}. \end{cases} \quad (2.6)$$

We see that for any t the function $y(x, t)$ defines one-to-one mapping (2.6) of $(0, 1)$ to some interval. All these formulas follow from results in Section 3 by simple scaling $x_k(t) \rightarrow \frac{1}{N}x_{\frac{k}{N}}(t)$.

Problem with Eulerian velocities. We could define the velocity $v(y, t)$ of “particle” which at moment t is situated at the point y by using the velocity of particle $x_k(t)$ closest to x from the left as follows (for any $c > 0$)

$$v(y, t) = \lim_{N \rightarrow \infty} \frac{x_k(t + \frac{c}{N}) - x_k(t)}{\frac{c}{N}},$$

but this will not have limit in the region where density $\rho(y, t) = 2$, as the velocity of particles $x_k(t)$ quickly fluctuates between 1 and -1 , as we will see below.

That is why we should increase the scale. namely, choose the corresponding particle $x_k(t)$ and define limiting velocities say on a bit greater scale - between 1 and $\frac{1}{\sqrt{N}}$ - for example on the scale $\frac{1}{\sqrt{N}}$ as:

$$v(y, t) = \lim_{N \rightarrow \infty} \frac{x_k(t + \frac{1}{\sqrt{N}}) - x_k(t)}{\frac{1}{\sqrt{N}}}$$

Then we get

Theorem 3. *For $0 < t < \frac{1}{2}$, $\frac{1}{2} < t < 1$ and $t > 1$ we have correspondingly*

$$v(y, t) = \begin{cases} 0, & 0 < y < t, \\ -1, & t < y < 1 - t, \\ 0, & 1 - t < y < 1, \end{cases} \quad v(y, t) = \begin{cases} 0, & 0 < y < 1 - t, \\ 1, & 1 - t < y < t, \\ 0, & t < y < 1, \end{cases}$$

$$v(y, t) = \begin{cases} 0, & 1 < y < t, \\ 1, & t < y < t + 1, \\ 0, & t + 1 < y, \end{cases}$$

3. Proofs – Cellular Automata and Words

Here we consider initial conditions (2.3).

Lemma 1. *At time moments $t \in D = \{\frac{j}{2} : j \in Z_+\}$ the particles can be only at the points $x \in D$. Moreover, at any time $t \in D$ and for any $1 < k \leq N$ the distance $x_k(t) - x_{k-1}(t)$ is either 1 or 0.*

These assertions will be clear from the constructions below.

In our case terminology of discrete mathematics (cellular automata, words) can help. Namely, we consider cellular automaton, where cells are numerated by numbers $i \in Z_+$ and the state of the cell i at time t is denoted by $\omega(i, t)$. Time is discrete $t \in D = \{\frac{j}{2} : j \in Z_+\}$, thus the time unit is $\frac{1}{2}$.

Each cell can be in only one of the 4 states $0, \pm 1, 2$. The state of all system (of our cell automaton with $2N$ cells) at time t we represent by the word (that is by finite sequence) of some length $n + 1$.

$$w(t) = \omega(0, t)\omega(1, t) \dots \omega(n, t),$$

that is by the sequence of states of all cells. But we will have in mind that $\omega(n, t) \neq 0$ and $\omega(i, t) = 0$ for $i > n$.

We will need below the following three words

$$w_{-,m} = 0(-1)0(-1) \dots 0(-1), \quad w_{+,m} = 0101 \dots 01, \quad w_{2,m} = 0202 \dots 02$$

Each of them has length $2m$ and consists of m repeated pairs $0(-1), 01, 02$ correspondingly. Each state of our automaton will consist of 1 or 2 of these words.

We will see that, in the dynamics, the state $\omega(i, t + \frac{1}{2})$ depends only on the states $\omega(i - 1, t)$ and $\omega(i + 1, t)$. More exactly the dynamics will be defined below. Thus one can also say that such dynamics defines deterministic locally interacting process.

Now we give exact relation of this cell automaton with our particle system. Namely, our main assumption above was that the initial velocities are equal and initial distances between particles are also equal. Remind that to make this relation more clear we use the scale (2.3). Then we want to describe the set $\{x_k(t)\}$ of particle trajectories in more detail. Note, that for any t the order of particles is conserved, that is $x_k(t) \leq x_{k+1}(t), k = 1, 2, \dots, N - 1$. This follows from the definition of dynamics.

We identify the cell i of the automaton with the point $\frac{i}{2} \in D$. and the sequence of cells with the sequence of these points The state of these cells is defined by the number of particles in this point and their velocities. Namely, we will see later that at any point can be either:

- 1) 0 particles (state 0);

- 2) 1 particle with velocity 1 (state 1) or -1 (state -1);
- 3) 2 particles, where one particle has velocity 1 and the other -1 (moment of collision).

We will need the following notation:

- 1. $X(t)$ – the maximal coordinate among the coordinates of collision points at time moment $t \in D$;
- 2. T_k – the time of first collision of the particle k . Note that the particle N can collide only with particle $N-1$. Thus, at the moment T_N particles $N-1, N$ will get velocities $-1, 1$ correspondingly;
- 3. X_k – the coordinate of the first collision of particle k ;
- 4. T_{NN} – the time when particle N will return to its initial position N ;
- 5. $k(x, t)$ – the (serial) number of the particle which has positive velocity at point x at time t , if there is such. Put $K(t) = k(X(t), t)$.

After scaling like in the theorems 1,2: 1) $x_N(t)$ defines the length of our “shock wave”. 2) $X(t)$ defines the trajectory of the boundary between domains with densities 1 and 2, 3) T_N defines the time when after permanent decrease of the length it becomes to increase.

There are 3 useful ways to understand the situation in detail. The first way – from the very beginning to see the increase of $X(t)$, 2) to understand the decrease of any $x_k(t)$ until T_k, X_k , 3) to imagine the whole picture in terms of cellular automaton. These ways correspond to the following lemmas.

Dynamics of the length.

Lemma 2. 1) If $t \leq T_N$ then

$$X(t) = t - 1, \quad K(t) = 2t - 1, \quad T_N = \frac{N+1}{2}, \quad X(T_N) = \frac{N-1}{2},$$

$$x_N(t) = N - t.$$

2) If $T_N < t < T_{NN}$ then

$$T_{NN} = N + 1, \quad X(t) = X(T_N) - (t - T_N) = N - t,$$

$$x_N(t) = X(T_N) + (t - T_N) = t - 1.$$

It is useful to start with initial steps. Initially ($t = 0$) we have the sequence of particles with all velocities -1 and with coordinates $1, 2, \dots, N$. This corresponds to the word $w(0) = 0\omega_{-,N}$ of length $2N + 1$ with $N + 1$ zeros and N cells with the state -1 .

At time $t = \frac{1}{2}$ we will have the word $w(\frac{1}{2}) = \omega_{-,N}$ of length $2N$. The first collision will occur when the particle 1 will reach the wall – that is at time $t = 1$. All other particles will have the integer coordinates $1, 2, \dots, N-1$. Thus at time $t = 1$ the particle 1 will get velocity $v_1(1) = 1$, and particle 2 at this moment

will be at the point 1 and will have velocity $v_2(1) = -1$. Particles 3, 4... will move to the left on the distance $\frac{1}{2}$. Thus at time $t = 1$ we will have the word $w(1) = 1w_{-,N-1}$ of length $2N - 1$.

At time $t = 1 + \frac{1}{2}$ particles 1 and 2 collide at the point $x = \frac{1}{2}$, at the same moment particle 3 will be at the point $x = \frac{3}{2}$. The corresponding word is $w(1 + \frac{1}{2}) = 02w_{-,N-2} = w_{2,1}w_{-,N-2}$.

At time $t = 2$ particle 1 will again collide with the wall and particles 2 and 3 collide at $x = 1$. That is $w(2) = 1w_{2,1}w_{-,N-3}$.

Thus we have the following sequence of words

$$w(0) = 0w_{-,N}, \quad w\left(\frac{1}{2}\right) = w_{-,N}, \quad w(1) = 1w_{-,N-1},$$

$$w\left(\frac{3}{2}\right) = w_{2,1}w_{-,N-2}, \quad w(2) = 1w_{2,1}w_{-,N-3}.$$

At moment $\frac{3}{2}$ there are two particles with numbers 1 and 2 at the point $\frac{1}{2}$. And particle with number 2 will have positive velocity. Other particles will be at the points

$$x_1\left(\frac{3}{2}\right) = x_2\left(\frac{3}{2}\right) = X\left(\frac{3}{2}\right) = \frac{1}{2},$$

$$x_3\left(\frac{3}{2}\right) = \frac{1}{2} + 1,$$

$$x_k\left(\frac{3}{2}\right) = \frac{1}{2} + k - 2, \dots,$$

$$x_N\left(\frac{3}{2}\right) = \frac{1}{2} + N - 2.$$

That is for $2 < k < N$

$$x_k\left(\frac{3}{2}\right) - x_{k-1}\left(\frac{3}{2}\right) = 1$$

Then $X\left(\frac{3}{2}\right) = \frac{1}{2}, K\left(\frac{3}{2}\right) = 2$, At the next moment $t = 2$ the particles 2 and 3 collide at point 1, and points with $k > 3$ will move to the left on $\frac{1}{2}$ without any collisions.

For any $t < T_N$ we will define a “quasiparticle” (leader) with trajectory $y(t), \frac{3}{2} \leq t$. Namely, on the interval $\frac{3}{2} \leq t < 2$ it is the particle 2, that is $y(t) = x_2(t)$. Then at time $t = 2$ particle 2 collides with particle 3 and passes leadership to it, that is on the time interval $2 < t \leq \frac{5}{2}$ it will be $y(t) = x_3(t)$. And so on: we can continue because no particle behind $y(t)$ cannot influence (cannot catch it up) its movement, as all velocities are ± 1 . In general at time moments $t \in D$ $y(t) = X(t)$ and it passes leadership to $k(X(t) + 1, t)$. Until $t = T_N$. After this particle N will move freely to the right with velocity 1. So,

$$X(t) - X\left(t - \frac{1}{2}\right) = \frac{1}{2}, \quad K(t) - K\left(t - \frac{1}{2}\right) = 1,$$

$$X\left(\frac{3}{2} + \tau\right) = \frac{1}{2} + \tau, \quad K\left(\frac{3}{2} + \tau\right) = 2 + 2\tau,$$

or putting $\frac{3}{2} + \tau = t$

$$X(t) = t - 1, \quad K(t) = 2t - 1 = 2X(t) + 1, \quad K(t) - X(t) = t.$$

Particle trajectories. Let T_k^+ be the smallest time after which particle k has always velocity 1, and $X_k^+ = x_k(T_k^+)$.

Lemma 3. For any particle k there are 3 stages of dynamics:

- 1) Particle k moves with velocity -1 until its first collision at time $T_k = \frac{k-1}{2}$;
- 2) It performs fluctuations with period $\frac{1}{2}$ in the time interval $T_k < t < T_k^+$. It fluctuates between two points X_k and $X_k + \frac{1}{2}$. Moreover, fluctuations of all fluctuating particles are synchronized, as it is shown in lemma 4,
- 3) It moves with velocity 1 for $t > T_k^+$.

Particle $x_N(t)$ has velocity -1 until its first collision, that is for $t < T_N$, and gets velocity 1 at the moment T_N . And has velocity 1 always afterwards that is for $t > T_N$, because no other particle can reach it.

Then $T_{N-1} = T_N - \frac{1}{2}$ as until time T_{N-1} (when particle $N - 1$ gets velocity 1) the distance between particles N and $N - 1$ is always 1.

Note that for any $k < N$ the particles $k, k + 1, \dots, N$ move with velocity -1 until the first collision of particle k . At the moment of first collision particle $k = k(X(t), t)$ gets velocity 1, and then, in one time unit, $X(t)$ increases on $\frac{1}{2}$ because

$$x_{k(X(t),t)+1} - x_{k(X(t),t)} = 1$$

and these subsequent particles collide at the point $x_{k(X(t),t)} + \frac{1}{2}$.

It follows by induction that

$$T_k = T_N - \frac{N - k}{2} = \frac{N + 1}{2} - \frac{N - k}{2} = \frac{k + 1}{2}. \tag{3.1}$$

In particular, the first collision of particle 1 (with the wall) is at time $T_1 = 1$.

Similarly,

$$\begin{aligned} X_N &= N - T_N = \frac{N - 1}{2}, \\ X_k &= k - T_k = \frac{k - 1}{2}. \end{aligned} \tag{3.2}$$

Particle k has its first collision with particle $k - 1$ and the second collision with particle $k + 1$. Afterwards it will have collisions with these two particles. Moreover, it will move back and forth between two points. Particle 1 fluctuates between points 0 and $\frac{1}{2}$, particle 2 - between $\frac{1}{2}$ and 1, particle 3 - between 1 and $\frac{3}{2}$, particle k - between points $\frac{k-1}{2}$ and $\frac{k}{2}$.

Dynamics of words.

Lemma 4. *In our dynamics there can be only the following 2 types of words (where $l \in Z_+$): 1) for $0 \leq l \leq \frac{N}{2}$ only*

$$w(N, l, -) = w_{2,l}w_{-,N-2l} \quad \text{and} \quad w_1(N, l, -) = 1w_{2,l}w_{-,N-2l-1},$$

2) for $\frac{N}{2} < l \leq N$ only

$$w(N, l, +) = w_{2,l}w_{+,N-2l} \quad \text{and} \quad w_1(N, l, +) = 1w_{2,l}w_{+,N-2l-1}.$$

The dynamics for unit of time $\frac{1}{2}$ in case 1) is

$$w_{2,l}w_{-,N-2l} \rightarrow 1w_{2,l}w_{-,N-2l-1} \rightarrow w_{2,l+1}w_{-,N-2l-2}.$$

In case 2) the dynamics is

$$w(N, l, +) = w_{2,l}w_{+,N-2l} \rightarrow 1w_{2,l-1}w_{+,N-2l+1} \rightarrow w_{2,l-1}w_{+,N-2l+2}.$$

We could equivalently write down dynamics in terms of real time if we put $l = 2t \iff t = \frac{l}{2}$.

Assume that at time t we have the word $w(t) = w_{2,l}w_{-,N-2l}$. Then l integer coordinates $0, 1, \dots, l-1$, will be empty and coordinates $\frac{1}{2}, \frac{3}{2}, \dots, \frac{2l-1}{2}$ will be collision points. It follows that

$$X(t) = l - \frac{1}{2}, K(t) = 2l.$$

As for the word $w_{-,N-2l}$, its corresponding coordinates $l, \dots, N-l$ will be empty and any of the same number of non-integer points contains one particle only.

We will show that at time $t + \frac{1}{2}$ the state of the system corresponds to the word

$$w(t + \frac{1}{2}) = 1w_{2,l}w_{-,N-2l}.$$

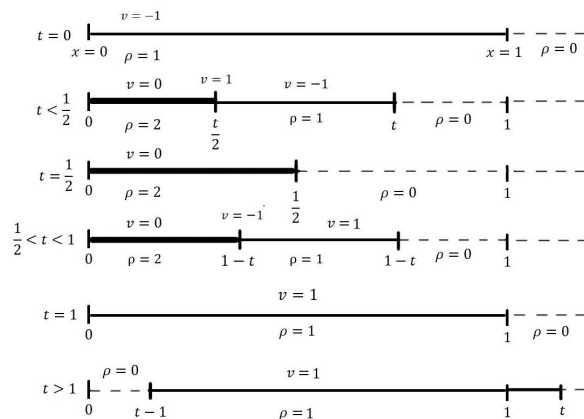
In fact, at time $t + \frac{1}{2}$ particle 1 will move to point 0, other integer points $1, 2, \dots, l$ will become collision points and non-integer points will become empty. A special case is the contact between particles $2l$ and $2l + 1$. The distance between them is 1, and their velocities are $v_{2l} = 1, v_{2l+1} = -1$. They collide and as a result, the points $X(t) = l - \frac{1}{2}$ and $X(t) = l + \frac{1}{2}$ become empty and the point l becomes a collision point.

Scaling. As $N \rightarrow \infty$ then in our scaling the main parameters change as follows:

- 1) $T_N \rightarrow \frac{1}{2}, T_{NN} \rightarrow 1$;
- 2) $X(t)$ becomes the point between left interval where $\rho = 2$ and right interval where $\rho = 1$. Thus, $X(t) \rightarrow t$ for $t \leq \frac{1}{2}$, and $X(t) \rightarrow 1 - t$ for $\frac{1}{2} < t < 1$;
- 3) if for example $k = [\alpha N]$, where $0 < \alpha < 1$, then $X_k \rightarrow \alpha$. Moreover, both T_k and X_k tend to $\frac{\alpha}{2}$.

4. Pictures

Here we show how the region of double density (thick segments) moves in time.



5. Conclusion

Other Problems There are many generalizations of our model - from simple to sufficiently difficult. First generalizations are of course initial conditions (2.1,2.2) but with non-equal distances between neighbors and/or non-equal velocities.

Remark 2. In our model below there was no simultaneous collisions of 3 or more particles at one point. But for other initial conditions this could occur and there are two ways to deal with this:

- 1) just ignore this problem, as such collisions can occur only for initial conditions from a subset G of R_+^{2N} with Lebesgue measure 0,
- 2) one can define somehow the distribution of velocities in such multiple collisions satisfying conservation laws.

But main generalization could be existence of external forces on some particles and various interactions between particles. One of the question is the convergence to known and unknown one-dimensional PDE of continuous mechanics. Note that we did not find this in our model. This indicates on the possibility that in some cases the situation cannot be described by accustomed PDE equations.

Below we give references to earlier work in this direction. But in our paper there are some new points:

1. Dynamics of particles at discrete time moments exactly coincides with the dynamics of cellular automaton.

2. Moreover, trajectories of particles are given explicitly. However, they are smooth only on some time intervals, depending on the initial position of the particle.

3. Density of particles has very strong gap, which also moves.

4. In our scaling $\frac{1}{N}$ the trajectories of particles tend to continuum dynamics trajectories. Nowever, velocities do not have limits in this scaling (due to local fluctuations of particles in the domain of double density), but do have for more rough scaling $\frac{1}{N^{1-\epsilon}}$.

More detailed mathematical review of earlier and possible future activity in this direction is in progress.

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