Visualization of the application of the discontinuous particle method without taking into account the particle shape to the quasi-linear transport equation

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<u>Abstract</u>

The paper considers a new variant of the discontinuous particle method. The main feature of the new variant is minimal smearing of discontinuities, due to the new criterion of rearrangement of particles. In contrast to the previously used variant with the analysis of overlaps of particles, which required an assumption about their shape, we use the key characteristic of particles, namely, their mass. The assumption is made that in nonlinear elastic transport not only the masses of the particles are conserved, but also the mass located between the centers of these particles. This requirement leads to the fact that a change of distance between particles in the process of their shear and conservation of mass in the space between them, lead to a change of density of one of the particles. The new version applies to solving the one-dimensional and two-dimensional quasi-linear transport equation problem. Visualization is used to monitor the numerical solution, showing that the shock velocity is calculated correctly, and the shock itself is smeared on one particle.

Keywords: particle method, inviscid Burgers' equation.

1 Introduction

The main feature of gas dynamics is the appearance of discontinuities, more precisely, strong gradients. The quality of computational methods is assessed primarily by their ability to convey this behavior of a solution as adequately as possible. In our opinion, the discontinuous particle method [1-3] allows one to cope with these difficulties better than alternative, traditionally more commonly used difference and finite element methods. This is achieved because the particle method is based on the Lagrange approach, and this, in turn, provides automatic mesh generation. In addition, particle methods have a constructive inclination to parallelization, economical from the point of view of multidimensionality, ideologically organic to hierarchical transitions between micro-macro models of the considered phenomena. It is worth noting that the problems of evaluating the accuracy of numerical methods on discontinuities currently are very relevant [4, 5].

The Burgers equation [6, 7], viscous and inviscid, is the simplest model, which shows the key feature for the whole gas dynamics: the existence of zones with strong gradients of the solution. Having correctly numerically simulated such zones, one can expect to build effective computational methods, not only and not so much for macro-models, but also for meso - levels of the hierarchy in the representation of the Kolmogorov – Fokker - Planck equations [1, 8, 9].

Using the terminology of Hockney and Eastwood [10], we divide the whole set of particle methods into 3 subclasses: particle-grid (PM) methods, particle-particle method (PP) and hybrid particle-particle - particle-grid methods (PPPM or P3M). In this classification, the discontinuous particle method can be classified as a particle-particle method. The smoothed

particle hydrodynamics method and its numerous modifications [11] or the material point method [12] belong to the same subclass. The particle method is used to solve problems in plasma physics and gas dynamics [10, 13, 14].

2 The basis of Discontinuous particle method

Let us assume there be *N* material points located at the initial time in coordinates x_i^0 and moving with velocities $v_i(x, t)$ (i = 1, ..., N). This verbal formulation corresponds to the Cauchy problem:

$$\begin{cases} \frac{\mathrm{d}x_{i}(t)}{\mathrm{d}t} = v_{i}(x_{i}(t), t), \\ x_{i}(0) = x_{i}^{0}, \quad i = 1, \dots, N. \end{cases}$$
(1)

This problem is a micromodel of the transport process. Let us show that one can pass from Eq. (1) to a macromodel of the linear transport process.

We determine the distribution density u(x, t):

$$u(x,t) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i(t)),$$
(2)
 $\forall \varphi(x) \in C_0^2 : \int \varphi(x) u(x,t) dx = \frac{1}{N} \sum_{i=1}^{N} \varphi(x_i(t)).$

The article [2] shows the transition from (1) and (2) to the generalized transport equation:

$$\int \varphi(x) \left(\frac{\partial u}{\partial t} + \frac{\partial v u}{\partial x} \right) dx = 0$$
(3)

and then to the transport equation in differential form:

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} + \frac{\partial (v(x,t)u(x,t))}{\partial x} = 0, \\ u(x,0) = u_0(x). \end{cases}$$
(4)

That is, if the coordinates of points change according to the system of equations (1), then the density u(x, t) is a generalized solution of the Cauchy problem for the transport equation (4). Instead of equation (4) we solve the system of equations (1). We can say that using the representation of the desired function as a set of δ -functions. What follows is an approximation of the δ -functions by classical functions, with which the calculations at each time step are performed.

Now write down another ODE system:

$$\begin{cases} \frac{\mathrm{d}x_{i}(t)}{\mathrm{d}t} = \frac{u_{i}(x,t)}{2}, \\ \forall \varphi(x) \in C_{0}^{2} : \int \varphi(x)u(x,t)\mathrm{d}x = \frac{1}{N} \sum_{i=1}^{N} \varphi(x_{i}(t)), \\ x_{i}(0) = x_{i}^{0}, \quad i = 1, \dots, N. \end{cases}$$
(5)

Making a transition from (5) similar to that for system (1), we obtain a one-dimensional quasi-linear transport equation:

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} + \frac{\partial \left[\frac{u(x,t)}{2}u(x,t)\right]}{\partial x} = 0, \\ u(x,0) = u_0(x). \end{cases}$$
(6)

Let's write down yet another ODE system:

$$\begin{cases} \frac{dx_{i}^{u}(t)}{dt} = u\left(x_{i}^{u}(t), y_{i}^{u}(t), t\right), \quad i = 1, ..., N_{u}; \\ \frac{dy_{i}^{u}(t)}{dt} = v\left(x_{i}^{u}(t), y_{i}^{u}(t), t\right), \quad i = 1, ..., N_{u}; \\ \frac{dx_{i}^{v}(t)}{dt} = u\left(x_{i}^{v}(t), y_{i}^{v}(t), t\right), \quad i = 1, ..., N_{v}; \\ \frac{dy_{i}^{v}(t)}{dt} = v\left(x_{i}^{v}(t), y_{i}^{v}(t), t\right), \quad i = 1, ..., N_{v}, \\ \forall \psi(x, y) \in C_{0}^{2} : \int \psi(x, y)u(x, y, t)dxdy = \frac{1}{N_{u}} \sum_{i=1}^{N} \psi(x_{i}^{u}(t), y_{i}^{u}(t)), \\ \forall \psi(x, y) \in C_{0}^{2} : \int \psi(x, y)v(x, y, t)dxdy = \frac{1}{N_{v}} \sum_{i=1}^{N} \psi(x_{i}^{v}(t), y_{i}^{v}(t)), \\ \forall \psi(x, y) \in C_{0}^{2} : \int \psi(x, y)v(x, y, t)dxdy = \frac{1}{N_{v}} \sum_{i=1}^{N} \psi(x_{i}^{v}(t), y_{i}^{v}(t)), \\ x_{i}^{u}(0) = x_{i}^{u,0}, \quad i = 1, ..., N_{u}, \\ y_{i}^{u}(0) = y_{i}^{u,0}, \quad i = 1, ..., N_{v}, \\ y_{i}^{v}(0) = y_{i}^{v,0}, \quad i = 1, ..., N_{v}, \\ y_{i}^{v}(0) = y_{i}^{v,0}, \quad i = 1, ..., N_{v}. \end{cases}$$

$$(7)$$

Similarly, it leads to a two-dimensional quasi-linear transport equation:

$$\begin{cases} \frac{\partial u(x, y, t)}{\partial t} + \frac{\partial u(x, y, t)u(x, y, t)}{\partial x} + \frac{\partial v(x, y, t)u(x, y, t)}{\partial y} = 0, \\ \frac{\partial v(x, y, t)}{\partial t} + \frac{\partial u(x, y, t)v(x, y, t)}{\partial x} + \frac{\partial v(x, y, t)v(x, y, t)}{\partial y} = 0, \\ u(x, y, 0) = u_0(x, y), \\ v(x, y, 0) = v_0(x, y). \end{cases}$$
(8)

In this section, we obtain the basic equations to which our method will later be applied.

3 Particle method using shapeless particles

Let us describe the discontinuous particle method for one-dimensional quasi-linear transport equation. Let's introduce the following notations: x_i^k is the coordinate of center of ith particle at k-th moment of time, v_i^k is the velocity of particle, h_i^k is the height (density) of particle, S_i is the area (mass) of particle. In previous works [1–3, 15] we also introduced w_i^k . This was the width of a particle. But now we consider particles shapeless, and we will not use this concept. For better perception, all these values are marked in Figure 1.



Figure 1: The main parameters used by the discontinuous particle method.

Let us assume that \tilde{S}_i^k is the area of the trapezium, whose bases are the heights of i-1 and i particles and whose sides are the distances between the particles, is constant.

$$\widetilde{S}_{i}^{k} = \frac{h_{i}^{k} + h_{i-1}^{k}}{2} \left(x_{i}^{k} - x_{i-1}^{k} \right)$$

Let the centers of the particles satisfy the ODE system (5). We solve the differential part of the system numerically using the explicit Euler scheme:

$$x_i^{k+1} = x_i^k + \tau \frac{u_i^k}{2}, i = 1, \dots, N.$$

Since the equation is nonlinear, the particles move at different speeds, as a result of which the area of the trapezoid between the particles can either increase or decrease. Taking advantage of the fact that the area of the trapezoid must remain constant, we write:

$$h_{i}^{k+1} = \frac{\left(h_{i}^{k} + h_{i-1}^{k}\right)\left(x_{i}^{k} - x_{i-1}^{k}\right)}{x_{i}^{k+1} - x_{i-1}^{k+1}} - h_{i-1}^{k}$$

Let's show this visually in Figure 2:



Figure 2: Visualizing the condition of constant trapezoidal area

However, we should keep in mind that by changing the height of a particle to preserve the area of one trapezium we have implicitly increased the area of the neighboring trapezium. To avoid the effect of such an implicit increase, we introduce an additional restriction: if *i*-*i*-th particle is higher than *i*-th, the area of the trapezium must decrease. And if it increases, the particles should not interact. If *i*-*i*-th particle is lower than *i*-th, the area of the trapezium must increase. And if the area decreases, the particles also do not interact. We can rewrite the condition of interaction of particles as follows:

$$\left(\widetilde{S}_{i}^{k}-\widetilde{S}_{i}^{0}\right)\left(h_{i}^{k}-h_{i-1}^{k}\right)>0$$

Next, we proceed to a description of the algorithm in the two-dimensional case. Using the aiming parameter from [3], we find a pair of interacting particles. As shown in Figure 3, we construct a trapezoid and pass from the solution of the two-dimensional problem to the one-dimensional one, which has already been described earlier.



Figure 3: Converting two-dimensional problem to a one-dimensional

It is worth noting that in the two-dimensional case the comparison with the trapezoidal area in real time is a certain difficulty. One can either store all data from the first time step and calculate old areas each time, or calculate all possible pairs of areas in advance, store them in a two-dimensional array, and then retrieve them as needed. Detailed comparative calculations have not been carried out, but it can be assumed that for a large number of particles with a small number of calculation time steps, the first option is advantageous. In the opposite case, it is preferable to use the second option.

This section shows the essence of the discontinuous particle method algorithm without explicitly using the particle form. This is how the initialization of variables and their subsequent changes are carried out in the program.

4 Numerical Examples

First, we solve the Cauchy problem for the one-dimensional quasi-linear transport equation (5) with initial conditions:

$$u_0(x) = \begin{cases} 2, & x \le 2.1, \\ 0.5, & x > 2.1. \end{cases}$$
(9)

There is an exact solution for such an initial condition:

$$u(x,t) = \begin{cases} 2, & x \le 2.1 + 1.25t, \\ 0.5, & x > 2.1 + 1.25t \end{cases}$$



Figure 4: Solution of the one-dimensional quasi-linear transport equation by the particle method.

Figure 4 shows animated visualization of the numerical solution of equation (5) with initial conditions (9). The red line shows the exact solution. It can be seen that the shock velocity is calculated correctly, the shock is smeared on one particle. After the high particle with higher velocity "collides" with the low particle with lower velocity, the low particle grows to the height of the high particle. Thus, their speeds are compared, the low particle stops growing. In its turn it "collides" with the next particle.

Then we solve the Cauchy problem for the one-dimensional quasi-linear transport equation (5) with initial conditions:

$$u_0(x,y) = \begin{cases} 0.5, & x \le 2.1, \\ 2, & x > 2.1. \end{cases}$$
(10)

There is also an exact solution for such an initial condition:

by the particle method.

Figure 5 shows animated visualization of the numerical solution of equation (5) with initial conditions (10). The red line shows the exact solution. It can be seen that the solution in the form of rarefaction wave is calculated less accurately.

Then we numerically solve the Cauchy problem for the two-dimensional quasilinear transport equation (7) with initial conditions:

$$u_0(x, y) = v_0(x, y) = \begin{cases} 6, & x \le 1, y \le 1, \\ 4, & \text{otherwise.} \end{cases}$$

Figure 6: Motion animation of the numerical solution of the two-dimensional Cauchy problem by the particle method.

The discontinuity propagation in the two-dimensional problem is represented in the form of animation (Fig. 6). For ease of perception, the particles in Figure 6 are depicted as circles. It should be understood that the shape of the particles is not used anywhere in the algorithm itself. The exact solution is indicated as a thick black line. You can see in Figure 6 that particles with higher velocity collide with particles with lower velocity. Those taper, and a oneparticle wide gap is formed. This shows the low approximation viscosity of our method. The particles then continue to collide with each other, so that the gap moves at the velocity corresponding to the analytical solution. A visual representation of the moving process of the shock in the computational domain allows us to evaluate the properties of the used numerical method.

5 Conclusions

Thus, we have demonstrated the possibility of a new version of the discontinuous particle method that allows us to numerically simulate a system of two-dimensional quasi-linear transport equations with high accuracy, which is especially pronounced in examples with discontinuous solutions. The visualization of the solution allows us to see the advantages and disadvantages of the method more clearly.

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