The Finite-Volume-Particle Method for Conservation Laws

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Abstract

In the Finite-Volume-Particle Method (FVPM), the weak formulation of a hyperbolic conservation law is discretized by restricting it to a discrete set of test functions. In contrast to the usual Finite-Volume approach, the test functions are not taken as characteristic functions of the control volumes in a spatial grid, but are chosen from a partition of unity with smooth and overlapping partition functions (the particles), which can even move along prescribed velocity fields. The information exchange between particles is based on standard numerical flux functions. Geometrical information, similar to the surface area of the cell faces in the Finite-Volume Method and the corresponding normal directions are given as integral quantities of the partition functions.

After a brief derivation of the Finite-Volume-Particle Method, this work focuses on the role of the geometric coefficients in the scheme.

1 Introduction

The Finite-Volume-Particle Method (FVPM) is a new mesh-less method for the discretization of conservation laws. The motivation for developing a new method is to unify advantages of particle methods and Finite-Volume Methods (FVM) in one scheme.

On the one hand, particle methods are very flexible because they are mesh-free. The need for mesh-less methods typically arises if problems with time dependent or very complicated geometries are under consideration because then the handling of mesh discretizations becomes technically complicated or very time

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consuming. Fluid flow with structural interaction or fast moving boundaries like an inflating air-bag are of that kind for instance.

In gas and fluid dynamics, the SPH method [Mon92] has been successfully applied to problems with free boundaries. Recent developments in the area of mesh-less methods include the Finite-Mass Method (FMM) [Yse97, GLY] and the partition of unity method (PUM) [GS00].

The basic idea in the FVPM is to incorporate elements of the FVM into a particle method. Specifically, one wants to adopt the treatment of boundary conditions and the FVM concept of numerical flux functions in order to avoid numerical fit-parameters as in the artificial viscosity terms of SPH.

The brief derivation of the Finite-Volume-Particle Method in the following section shows that the scheme is essentially determined by the numerical flux function and a set of geometrical coefficients which play the role of normal directions and surface areas of cell faces in the Finite-Volume Method. For one-dimensional, scalar conservation laws, a Lax-Wendroff type consistency analysis and stability requirements lead to a set of conditions on the coefficients. For example, a CFL-type condition assures monotonicity of the scheme if the underlying numerical flux function is monotone. Numerical examples are presented to show the behavior of the scheme in the case of Burgers' equation. The extension to two-dimensional cases is demonstrated for the system of Euler equations. For certain 2D shock tube problems, it is shown how the identification of the geometric coefficients with their Finite-Volume counterparts (i.e. normal directions and length of cell faces) allows the implementation of boundary conditions.

2 Derivation of the scheme

In the following, we will briefly summarize the derivation of FVPM which was developed in [HSS]. As already mentioned above, FVPM is a numerical method for solving conservation laws of the type

$$\frac{\partial}{\partial t}\boldsymbol{\Phi}(t,\boldsymbol{x}) + \nabla \cdot \boldsymbol{F}(\boldsymbol{\Phi}(t,\boldsymbol{x})) = \mathbf{0}, \qquad \forall \boldsymbol{x} \in \Omega \subset \mathbb{R}^d,\, t \in \mathbb{R}^+ \tag{1}$$

with accompanying boundary and initial conditions $\boldsymbol{\Phi}(0,\boldsymbol{x}) = \boldsymbol{\Phi}^{(0)}(\boldsymbol{x})$. Here, $\boldsymbol{\Phi}$ denotes the vector of conservative variables, $\boldsymbol{F}$ is the flux function of the conservation law, d is the spatial dimension, and Ω is the domain under consideration.

A natural approach to discretize conservation laws is to evaluate the weak formulation with a discrete set of test functions $\psi_i, i = 1,..,N$. In classical Finite-Volume Methods, the test functions are taken as characteristic functions $\psi_i(\boldsymbol{x}) := \mathbb{I}_{\nu_i}(\boldsymbol{x})$ of the control volumes ν_i in a spatial grid. Note that the test functions form a *partition of unity*, i.e. $\sum_{i=1}^{N} \psi_i(\boldsymbol{x}) \equiv 1$, $\forall \boldsymbol{x} \in \Omega$.

In contrast to that, *smooth* test functions ψ_i (called *particles*) are employed in the FVPM. More precisely, at the *particle positions* $\boldsymbol{x}_i(t)$, the construction of

ψ_i is based on a compactly supported smoothing kernel $W(\boldsymbol{x})$, as it is used, for example, in the SPH method. The functions $W_i(\boldsymbol{x}) = W(\boldsymbol{x} - \boldsymbol{x}_i(t))$ are then re-normalized by the particle-density $\sigma(x)$, according to Shepard's method

$$\psi_i(t, \boldsymbol{x}) := \frac{W(\boldsymbol{x} - \boldsymbol{x}_i(t))}{\sigma(t, \boldsymbol{x})}, \quad \text{where} \quad \sigma(t, \boldsymbol{x}) := \sum_{j=1}^{N} W(\boldsymbol{x} - \boldsymbol{x}_j(t)).$$

For an illustration of the construction of the test functions ψ_i see Figures 1 to 3. Due to Shepard's re-normalization, the particles form a *partition of unity*

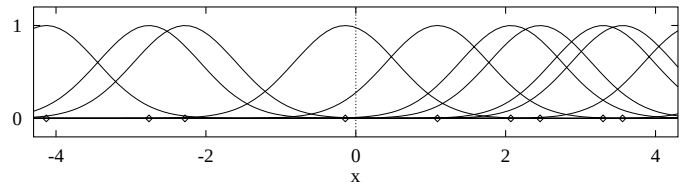

Figure 1: Irregular particle positions x_i and functions $W_i(x) = W(x - x_i)$

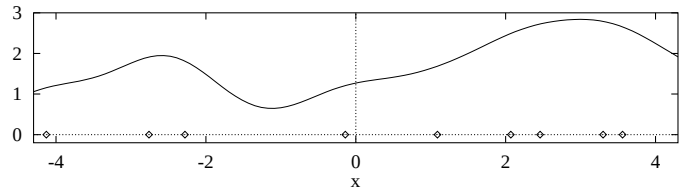

Figure 2: The function $\sigma(x) = \sum_i W_i(x)$ corresponding to Fig. 1

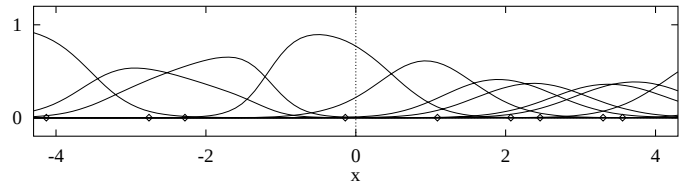

Figure 3: The resulting partition of unity $\psi_i(x) = W_i(x)/\sigma(x)$

similar to the characteristic functions of the control-volumes in the FVM. In Figure 3, one can see that the resulting test functions are scaled according to the particle-density, i.e. in regions where the particle-density is high the corresponding test functions are small which means small local weights of the corresponding particles.

In the FVPM, the particles generically move through the domain, following the 'arbitrary' velocity vectors $\boldsymbol{u}_i$, i.e. $\dot{\boldsymbol{x}}_i = \boldsymbol{u}_i$. For $\boldsymbol{u} = \boldsymbol{0}$, one obtains fixed particles and for $\boldsymbol{u}$ being, for example, the fluid velocity in the case of Euler equations, one obtains a Lagrangian scheme.

To each particle, one associates a volume V_i and a discrete quantity $\mathbf{\Phi}_i$ which is the integral mean value with respect to the test function

$$\mathbf{\Phi}_i(t,\boldsymbol{x}) := \frac{1}{V_i}\int\limits_{\Omega} \mathbf{\Phi}(t,\boldsymbol{x})\psi_i(t,\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \text{where} \quad V_i(t) := \int\limits_{\Omega} \psi_i(t,\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

Using the test functions and quantities defined above, one obtains the following evolution equations for the discrete quantities from the weak formulation of the Cauchy problem (1) (see [HSS] for details):

$$\frac{d}{dt}\left(V_i\mathbf{\Phi}_i\right) = -\sum_{j=1}^{N} |\boldsymbol{\beta}_{ij}|\tilde{\boldsymbol{F}}\left(\mathbf{\Phi}_i, \mathbf{\Phi}_j; \frac{\boldsymbol{\beta}_{ij}}{|\boldsymbol{\beta}_{ij}|}\right) + \sum_{j=1}^{N}\left(\boldsymbol{\gamma}_{ij}\cdot\dot{\boldsymbol{x}}_j\mathbf{\Phi}_i - \boldsymbol{\gamma}_{ji}\cdot\dot{\boldsymbol{x}}_i\mathbf{\Phi}_j\right), \quad (2)$$

together with

$$\frac{d}{dt}V_i = \sum_{j=1}^{N}\left(\boldsymbol{\gamma}_{ij}\cdot\dot{\boldsymbol{x}}_j - \boldsymbol{\gamma}_{ji}\cdot\dot{\boldsymbol{x}}_i\right), \qquad \frac{d}{dt}\boldsymbol{x}_i = \boldsymbol{u}_i.$$

The coefficients $\boldsymbol{\gamma}_{ij}$ and $\boldsymbol{\beta}_{ij}$ are defined as

$$\boldsymbol{\beta}_{ij} := \boldsymbol{\gamma}_{ij} - \boldsymbol{\gamma}_{ji}, \quad \boldsymbol{\gamma}_{ij} := \int \psi_i \frac{\nabla W_j}{\sigma}\,\mathrm{d}\boldsymbol{x}. \quad (3)$$

The right hand side of the evolution equation (2) consists of two parts. The first part is the flux term, where a standard numerical flux function $\tilde{\boldsymbol{F}}$ may be used, and the second term corresponds to the movement of the particles.

We remark that the formulation (2) may suffer from instabilities as can be seen by applying the discretization to the trivial scalar conservation law

$$\frac{\partial\Phi}{\partial t} = 0, \qquad \Phi(0,x) = H(x), \quad x\in\mathbb{R}$$

where H is the Heaviside function. We use the numerical flux $\tilde{F}\equiv 0$ and equidistant particles at $x_i = ih$, $i\in\mathbb{Z}$ which move with a common speed $\dot{x}_i = -1$. The hat function $W(x) = (1-|x/h|)_+$ then gives rise to $\psi_i(t,x) = W(x-x_i(t))$ since $\sigma\equiv 1$. With these choices, the scheme (2) reduces to

$$\frac{d\Phi_i}{dt} + \frac{\Phi_{i+1}-\Phi_{i-1}}{2h} = 0$$

which leads to the unconditionally unstable central scheme if the time derivative is discretized with a forward Euler method. Note that the central difference has its origin in the second sum in (2) which reflects corrections due to the movement of the particles.

A more stable discretization has been proposed in [JS00] where the movement terms are incorporated into the flux function, leading to a scheme of the form

$$\frac{d}{dt}\left(V_i \boldsymbol{\Phi}_i\right) = -\sum_{j=1}^{N} |\boldsymbol{\beta}_{ij}| \boldsymbol{G}_{ij} \tag{4}$$

where $\boldsymbol{G}_{ij}$ is a numerical flux function which corresponds to the modified flux $\boldsymbol{G}(t, \boldsymbol{x}, \boldsymbol{\Phi}) = \boldsymbol{F}(\boldsymbol{\Phi}) - \boldsymbol{\Phi} \otimes \boldsymbol{u}$. Selecting for example a flux function based on upwind ideas, we conclude that the example $\boldsymbol{F} \equiv \boldsymbol{0}$ no longer leads to instabilities since the movement terms are now treated properly.

3 The coefficients of the scheme

3.1 Formal aspects of the coefficients

The behavior of the FVPM is significantly influenced by the coefficients $\boldsymbol{\gamma}_{ij}$ and $\boldsymbol{\beta}_{ij}$ defined in (3). In order to analyze the effect of the coefficients, we consider the scheme (4) for scalar valued equations in $\Omega = \mathbb{R}$. Proofs for the results can be found in [HSS, JS00, Tel00].

A symmetry condition of the form

$$\beta_{ij} = -\beta_{ji} \tag{5}$$

ensures that the scheme is conservative, i.e. that $\frac{d}{dt}\left(\sum_i V_i \boldsymbol{\Phi}_i\right) = 0$. Monotonicity of the scheme follows under a CFL-like condition on the time-step if a monotone numerical flux function is used

$$L \frac{\Delta t}{\mathsf{min}_i V_i} < \frac{1}{\mathsf{max}_i \sum_j |\beta_{ij}|}. \tag{6}$$

Here, L is the Lipschitz constant for the numerical flux function which is related to the maximal characteristic speed in the problem. Furthermore, monotonicity and a summation condition of the form

$$\sum_{j \in \mathbb{Z}} \beta_{ij} = 0, \, \forall i \in \mathbb{Z}, \tag{7}$$

give $\mathbb{L}^\infty$-stability for finite times $0 \leq t \leq T$

$$\| \sum_i \Phi_i(t) \psi_i \|_{\mathbb{L}^\infty} \leq e^{CT} \| \sum_i \Phi_i(0) \psi_i \|_{\mathbb{L}^\infty}. \tag{8}$$

If the coefficients additionally satisfy a summation condition of the form

$$\sum_{i \geq i_0} \sum_{j \geq i_0} \beta_{ij} = 1 \tag{9}$$

the scheme is consistent in the sense of Lax-Wendroff, i.e. if the approximate solutions converge in a suitable sense, they converge to a weak solution.

An estimate for the total variation is in preparation and seems to be achievable under the conditions (6) and (7). To finally get convergence of the scheme to the entropy-solution, an entropy inequality is required.

We remark that conditions (7) and (9) are difficult to ensure if the integrals in (3) are evaluated numerically and that violation of these conditions may lead to instabilities of the method. To illustrate, for example, the effect of the summation-condition (7) on the scheme we consider a standard Riemann problem for Burgers' equation. In the left plot of Figure 4, the summation condition (7) is not fulfilled, which leads to unphysical oscillations in the constant part of the solution. In the right plot, the condition is satisfied and the oscillations vanish (see [Tel00] for the proof). Since highly accurate numerical integration is

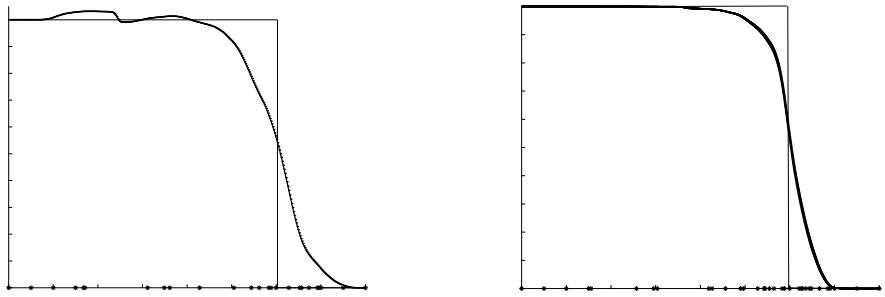

Figure 4: The effect of the summation condition (7) on the solution.

very time consuming, the determination of the coefficients turns out to be the most expensive part of the scheme. To alleviate this problem, a method has been proposed in [Tel00] which is based on a coarse evaluation of the integrals and a subsequent correction procedure in order to ensure (5), (7), and (9). However, this method is still at an experimental stage.

3.2 Heuristic interpretation of the coefficients

According to the definition (3), the coefficients $\boldsymbol{\beta}_{ij}$ are averaged, weighted, and symmetrized gradients of the smoothing kernels. This interpretation is illustrated in Figure 5. A formal comparison with standard Finite-Volume Methods (see (10) and (11)) indicates that the coefficients $|\boldsymbol{\beta}_{ij}|$ and $\boldsymbol{\beta}_{ij}/|\boldsymbol{\beta}_{ij}|$ can be interpreted as generalized surface area $|S_{ij}|$ of cell faces in the FVM and the corresponding

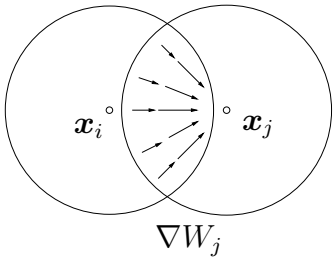

Figure 5: The gradient of the smoothing kernel: ∇W_j.

normal directions $\boldsymbol{\nu}_{ij}$:

$$\frac{d}{dt}(V_i \boldsymbol{\Phi}_i) = -\sum_j |\boldsymbol{\beta}_{ij}| \tilde{\boldsymbol{F}} \left(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j, \frac{\boldsymbol{\beta}_{ij}}{|\boldsymbol{\beta}_{ij}|} \right) \quad \text{FVPM } (\dot{\boldsymbol{x}}_i = \boldsymbol{0}), \tag{10}$$

$$\frac{d}{dt}(V_i \boldsymbol{\Phi}_i) = -\sum_j |S_{ij}| \tilde{\boldsymbol{F}}(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j, \boldsymbol{\nu}_{ij}) \qquad \text{FVM.} \tag{11}$$

These considerations indicate that the Finite-Volume-Particle Method is in some sense a 'generalization' of the standard Finite-Volume Method. In fact, the use of smooth and overlapping test functions (in contrast to the characteristic functions in the FVM) can be interpreted as a generalization of FVM to overlapping, smoothed, and moving control volumes.

4 Numerical results

The validation of the scheme is done by solving a standard and a modified 2D shock tube problem for the Euler equations of gas dynamics with free-slip boundary conditions.

4.1 Boundary treatment

The boundary treatment of the FVPM consists of two parts: Firstly, the boundary interacts with a particle by cutting off the support of the test function in definition (3) of the coefficients $\boldsymbol{\gamma}_{ij}$. Secondly, free-slip boundary-conditions are implemented using boundary-fluxes similar to the FVM.

The boundary-fluxes are computed using the normal $\boldsymbol{n}_i$ and the tangential vector $\boldsymbol{t}_i$ of the boundary at the corresponding particle $\boldsymbol{x}_i$ and the numerical flux function $\tilde{\boldsymbol{F}}(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_j; \boldsymbol{n}_i)$ which is used in the scheme. The auxiliary state $\boldsymbol{\Phi}_j$ is computed so that the boundary conditions are satisfied:

$$\boldsymbol{u}_i \cdot \boldsymbol{n}_i = -\boldsymbol{u}_j \cdot \boldsymbol{n}_i, \qquad \boldsymbol{u}_i \cdot \boldsymbol{t}_i = \boldsymbol{u}_j \cdot \boldsymbol{t}_i.$$

4.2 Quasi-1D shock tube problem

As initial condition, a density and pressure ratio of 1/10 across an initial shock at $x = 0.55$ in the domain $[0, 1] \times [0, 0.1]$ has been chosen. The shock front travels towards the right wall where it is reflected. The calculation is based on 1 000 particles (100 in x-direction and 10 in y-direction).

In Figure 6 a cut through the domain is shown. The density of the particles is plotted over the x-component of the position at time $t = 0.2$ and $t = 0.6$ in the left and right plot, respectively. Reflection of the shock wave at the right wall has already taken place in the right plot.

The simulation shows that the implementation of the boundary conditions works very satisfactory. No boundary effects are visible because all cuts through the domain give the same result.

In order to avoid holes in the computational domain by the movement of the particles, the radius of the particle support is chosen as $h = 1.8\Delta x$, where Δx denotes the initial distance between particle positions in x-direction.

Comparing FVPM and FVM based on the same flux function (Roe's flux), we find that despite the considerable overlap of the particles, the FVPM-solution turns out to be almost as accurate as the FVM-solution on a fixed 100×10 grid (spacing Δx) and it is notably better than the FVM-solution on a grid with spacing $2h$.

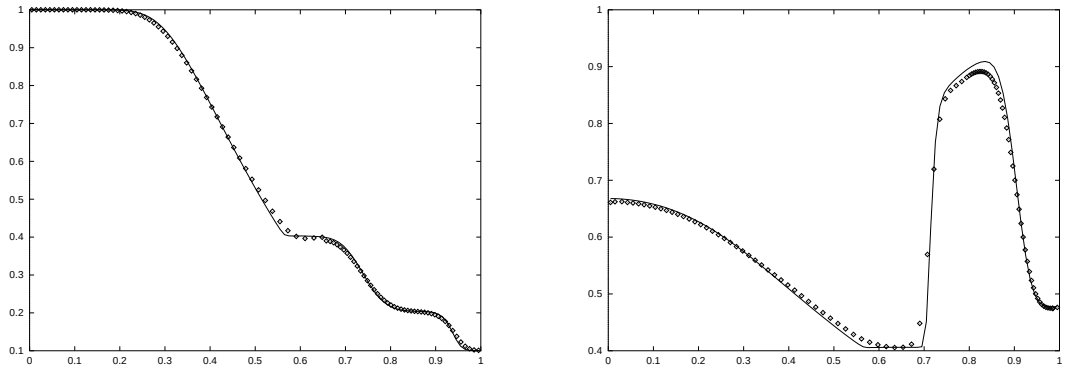

Figure 6: Solution of the standard shock-tube problem (density). Left: Before the shock front reaches the right wall at $t = 0.2$. Right: After reflection at the right wall at $t = 0.6$. The solid line is a FVM-solution on a 100×10 grid.

4.3 Modified shock tube problem

In the modified problem a quadratic domain is considered and the discontinuity in the initial data is located along the diagonal of the domain $x = y$. The shock front travels towards the upper left corner where it is reflected. Figure 7 shows the density and the velocity field shortly after reflection. The computation was performed on a domain $[0, 20] \times [0, 20]$ with 10 000 particles.

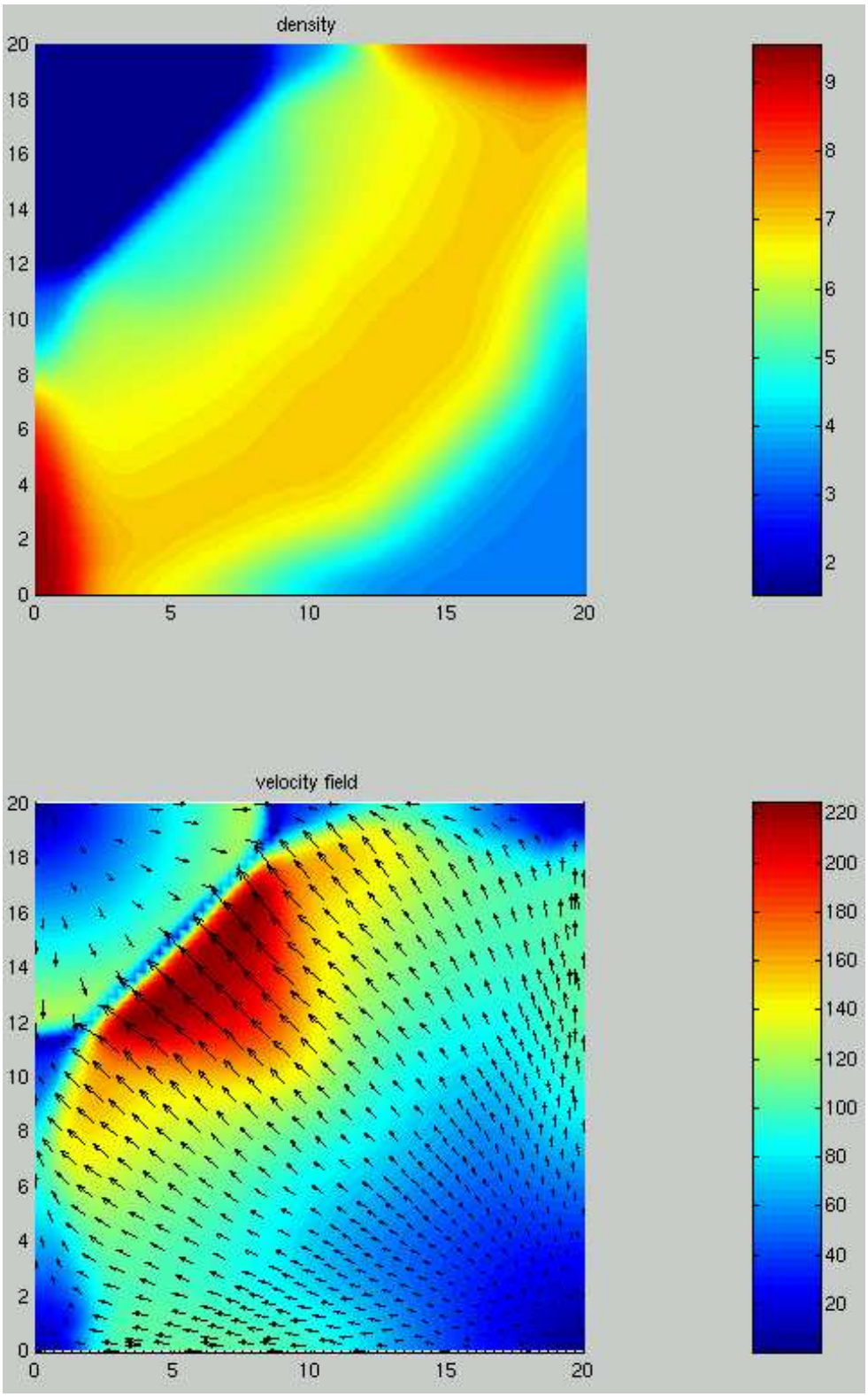

Figure 7: Solution of the shock problem after reflection in the upper left corner.

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