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FAST NUMERICAL METHOD FOR THE BOLTZMANN EQUATION ON NON-UNIFORM GRIDS

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ABSTRACT. We introduce a new fast numerical method for computing discontinuous solutions to the Boltzmann equation and illustrate it by numerical examples. A combination of adaptive grids for approximation of the distribution function and an approximate fast Fourier transform on non-uniform grids for computing smooth terms in the Boltzmann collision integral is used.

1. INTRODUCTION

This paper is devoted to a new deterministic scheme for numerical solution of the classical *Boltzmann equation* [10] for a dilute gas of particles.

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = Q(f, f), \tag{1.1}$$

where $f := f(t, \mathbf{x}, \mathbf{v})$ and $f : \mathbb{R}_+ \times \Omega \times \mathbb{R}^3 \to \mathbb{R}_+$. The collision operator Q is defined as follows

$$Q(f, f)(\mathbf{v}) := \int_{\mathbb{R}^3} \int_{S^2} B(|\mathbf{v} - \mathbf{w}|, \theta) \left[f(\mathbf{v}') f(\mathbf{w}') - f(\mathbf{v}) f(\mathbf{w}) \right] d\omega \, d\mathbf{w}, \tag{1.2}$$

where $\mathbf{v}$, $\mathbf{w}$ are the velocities of the particles before the collision and $\mathbf{v}'$, $\mathbf{w}'$ – the velocities of the particles after collision – are given by

$$\mathbf{v}' := \frac{1}{2} \left(\mathbf{v} + \mathbf{w} + |\mathbf{v} - \mathbf{w}| \omega \right), \qquad \mathbf{w}' := \frac{1}{2} \left(\mathbf{v} + \mathbf{w} - |\mathbf{v} - \mathbf{w}| \omega \right).$$

Moreover θ is the angle between the relative velocity $\mathbf{u} = \mathbf{v} - \mathbf{w}$ before and $\mathbf{u}' = \mathbf{v}' - \mathbf{w}'$ after collision.

The function $B(|\mathbf{v} - \mathbf{w}|, \theta)$ is of the form

$$B(|\mathbf{u}|, \theta) = B_0 \left(|\mathbf{u}|, \frac{|(\mathbf{u}, \omega)|}{|\mathbf{u}|} \right), \; u \in \mathbb{R}^3, \omega \in S^{(2)}, \; S^{(2)} = \{ \mathbf{q} \in R^3 : |\mathbf{q}| = 1 \}.$$

It contains the information about the binary interactions of particles and reflects the physical properties of the model.

The condition $B(|\mathbf{u}|, \cdot) \in L^1(S^{(2)})$, $\mathbf{u} \in \mathbb{R}^3$ is usually assumed to obtain separately convergent integrals for the positive "gain" and the negative "loss" parts in (1.2). For example if the particle interactions are modeled by inverse

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power forces with angular cut-off that means that grazing collisions do not take place, then

$$B_0(r, x) = r^\gamma b(x), \tag{1.3}$$

where $\gamma \in (-3, 1]$, and $b \in L^1([0, 1])$. In the case of "hard sphere" molecules, $B_0(r, x) = rx$.

In the case of popular Variable Hard Sphere model (VHS) the collision kernel B has the following form

$$B(|\mathbf{v} - \mathbf{w}|, \theta) = C_\alpha |\mathbf{v} - \mathbf{w}|^\alpha. \tag{1.4}$$

with $-3 < \alpha \leq 1$. For $\alpha = 0$ with $C_0 = \frac{1}{4\pi}$ we get the so called Maxwellian gas and for $\alpha = 1$ with $C_1 = 1$ we get the gas of hard spheres.

To solve the non-stationary Boltzmann equation numerically a splitting method in time is commonly applied.

At each time step in one solves first the *homogeneous Boltzmann equation*

$$\frac{\partial f}{\partial t} = Q(f, f) \quad \text{for all } \mathbf{x} \in \Omega \tag{1.5}$$

and then the *transport equation*

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = 0 \quad \text{for all } \mathbf{v} \in \mathbb{R}^3. \tag{1.6}$$

The main problem for the efficient numerical computations of the Boltzmann equation is a proper approximation of the collision operator $Q(f, f)$. We concentrate here mainly on the approximation of the collision operator in velocity space and hence demonstrate the method on examples with space homogeneous solutions. The application of the same approach for space dependent problems will be demonstrated in a subsequent paper.

In the next sections we will omit the dependence of f on the t and $\mathbf{x}$ variables for brevity where it is not confusing.

The numerical solution of the Boltzmann equation is difficult due to the nonlinearity of the collision integral, the large number of independent variables and the complicated integration over a five-dimensional cone in the six-dimensional space of pre and post collisional velocities. This analytical structure of $Q(f, f)$ implies that a straightforward computation of the collision integral by a standard quadrature has the computational cost N^3 for N points representing state of a gas in the velocity space. We point out that this is the cost of computations just in one point x in the physical space for a space non-homogeneous problem.

Particular symmetries of the collision operator imply conservation laws that in turn imply important connections between the Boltzmann equation and equations of classical gas dynamics.

Consequently the major part of practical applied computations concerning the Boltzmann equation is based on different variants of the probabilistic

Monte Carlo methods. Monte Carlo methods are advantageous for many high dimensional problems in physics, giving realistic and meaningful results with low computational cost proportional to the number N of particles (points) representing the system. On the other hand getting high precision results by Monte Carlo methods requires a higher computational time and for the number N_{tr} of stochastic trajectories they demonstrate low convergence order $\sqrt{N_{tr}}$. We refer to the direct simulation method (DSMC) by Bird [5] and to variants of Monte Carlo method for the Boltzmann equation by Nanbu [17] and Babovsky [3].

Development of deterministic methods for the Boltzmann equation is usually motivated, see [22], [18] by the desire of higher precision results, and by the existence of situations (low Knudsen numbers, slow convection flows) when probabilistic methods are not effective enough. Also not at the last place in the motivation of studies in this direction one finds the mathematical challenge of the problem itself.

We begin with a short discussion of the earlier results in the area of deterministic methods for the Boltzmann equation. Historically so called discrete velocity models (DVM) with uniform cubic grid of velocities were the first example of a numerical approach designed specially for the Boltzmann equation, starting from D. Goldstein, B. Sturtevant and J.E. Broadwell [12]. Later several different ideas led to other types of models all satisfying exact conservation laws in discrete form [23]. [9], [20].

Also rigorous consistency and convergence results for such models were proved [19], [16], [20].

Let n denote the number of points along one coordinate direction in the uniform velocity grid. All above mentioned DVM methods have high n^7 computational cost and have also a disadvantage that the integration over the sphere S^2 of the possible outputs of collisions in $Q(f, f)$ is approximated with low precision of order $1/\sqrt{n}$ [19]. In the case of the alternative so called Carleman formulation for $Q(f, f)$ this integration is substituted by the integration over some arbitrarily oriented planes with the same approximation problems [20]. It happens because only a small number of points from the uniform cubic grid meets spheres and arbitrarily oriented planes and these points are distributed not uniformly.

The Kyoto group in kinetic theory developed a family of finite difference methods for the Boltzmann equation, linearized Boltzmann equation, and the BGK equation and investigated numerically many mostly stationary problems [18],[14]. These computations demonstrate precise results but they are very time and memory consuming.

For computation of macroscopic flows with low Knudsen numbers so called lattice Boltzmann computational models with small (6 to 30 velocity points) are successfully applied, see [24] for references in this area. These simple

models have structure that reminds the Boltzmann equation but without the goal to approximate solutions to the last one. Also several larger simplified models of the collision operator $Q(f,f)$ were suggested recently, see for example [1] that do not approximate of the Boltzmann equation precisely but demonstrate somehow reasonable behavior of macro-parameters.

The simpler structure of the Boltzmann collision operator in the case of Maxwell pseudo molecules, by applying Fourier transform lets to reduce the collision operator to an expression with smaller dimension of the integration [7]. Using this reduction and the Fast Fourier Transform (FFT) led authors in [11] and [6] to a fast deterministic method restricted to Maxwell pseudo molecules and having low computational cost N^4 but still low accuracy $1/\sqrt{N}$. Here N is the number of Fourier modes along one coordinate direction. Another method designed for the model of hard spheres and also using FFT was suggested in [8] and has computational cost $N^6 \log N$ and a higher accuracy of order $1/N^2$.

A spectral method based on the restriction of the Boltzmann equation to a finite domain and on the representation of the solution by Fourier series was suggested in [21], and developed further in [22]. This method has an advantage of high spectral accuracy for smooth solutions to the Boltzmann equation and complexity N^6.

Any effort to develop a deterministic scheme for boundary value problems for the Boltzmann equation, includes as a necessary step computation of the collision operator $Q(f,f)$ for distribution functions typical for flows with boundaries. A typical distribution function for a gas close to the boundary has a discontinuity along a plane.

One observes easily that in a collisionless flow around a body the distribution function has a discontinuity in velocity space along a cone like surface that is built of the contour of the body seen from the point of observation. Computations done by the Kyoto group show that typical distribution functions for flows around a body have actually a similar discontinuity for a wide spectrum of Knudsen numbers [25].

It means that solutions to a boundary value problem are typically not smooth and Fourier based spectral approximations for them loose accuracy. The Gibbs phenomenon makes an alternative way of approximation necessary for such solutions.

To overcome this difficulty is the main goal of the present paper. One of the main ideas of the project comes from the classical result that the gain term $Q^+(f,f)$ in the collision operator has certain smoothing properties [15], [26] and therefore is smooth even for discontinuous f. One can illustrate this fact by the graph of $Q^+(f,f)$ in the x-z plane for a discontinuous function, see Figure 1. Collision frequency $q^-(f)$ is also a smooth function because it is a convolution of f with a regular function.

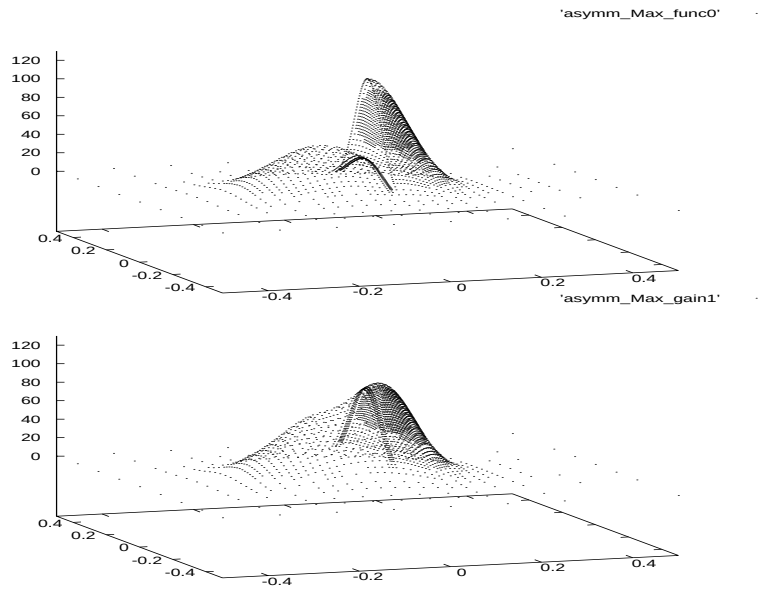

FIGURE 1. A distribution function f with discontinuity and the corresponding gain term $Q^+(f,f)$

We introduce here an approximation scheme that can effectively handle solutions to the Boltzmann equations discontinuous in velocity space. It is based on a new method for approximation of the Boltzmann collision operator and its solutions using non-uniform grids in velocity space. The following techniques make input to its computational efficiency:

i) Fourier based spectral representation of the gain part of collision operator as a bilinear pseudodifferential operator excluding effectively integration over spheres from numerical computations;

ii) effective resolution of discontinuities of solutions using an adaptive grid;

iii) high precision spectral representation for smooth terms in the Boltzmann equation;

iv) application of an approximate Fast Fourier transform on non-uniform grid for fast computation of the gain term and collision frequency on the adaptive grid;

v) an approximate algebraic decomposition of the symbol of the bilinear pseudodifferential expression for the gain term.

Techniques i) and iii) were used before, ii), iv), v) are new for the Boltzmann equation. The idea to combine a spectral representation for smooth terms in the Boltzmann equation with approximation on and adaptive grid for the discontinuous distribution function f is new. The combination of

adaptive grids with non-uniform Fast Fourier transform was previously used for approximation of geometric flows in [13].

2. Transformation of the collision integral

The collision operator (1.2) for potentials with angular cut off [10] can be decomposed into the *gain* and the *loss* parts

$$Q(f,f)(\mathbf{v}) = Q^+(f,f)(\mathbf{v}) - Q^-(f,f)(\mathbf{v}), \tag{2.1}$$

where

(2.2)

$$Q^+(f,f)(\mathbf{v}) = \int_{\mathbb{R}^3}\int_{S^2} B(|\mathbf{u}|,\theta) f(\mathbf{v} - \frac{1}{2}(\mathbf{u} - |\mathbf{u}|\omega)) f(\mathbf{v} - \frac{1}{2}(\mathbf{u} + |\mathbf{u}|\omega)\, d\omega\, d\mathbf{u}$$

and

$$Q^-(f,f)(\mathbf{v}) = f(\mathbf{v}) q^-(f)(\mathbf{v}) \tag{2.3}$$

with q^- denoting the *collision frequency* term

$$q^-(f)(\mathbf{v}) = \int_{\mathbb{R}^3} f(\mathbf{v}-\mathbf{u}) \int_{S^2} B(|\mathbf{u}|,\theta)\, d\omega\, d\mathbf{u}.$$

We have changed the variables $\mathbf{u} = \mathbf{v} - \mathbf{w}$ in the collision integral in (1.2) to get the above formulations.

We will use the following form of the Fourier transform

$$F_v(\mathbf{m})[f] := \hat{f}_m = \int_{\mathbb{R}^3} f(\mathbf{v}) e^{2\pi\imath(\mathbf{v},\mathbf{m})}\, d\mathbf{v} \tag{2.4}$$

and inverse Fourier transform

$$F_m^{-1}(\mathbf{v})[\hat{f}] := f(\mathbf{v}) = \int_{\mathbb{R}^3} \hat{f}_m e^{-2\pi\imath(\mathbf{m},\mathbf{v})}\, d\mathbf{m}. \tag{2.5}$$

Now we can reformulate the gain and collision frequency terms using the Fourier transform:

$$Q^+(f,f)(\mathbf{v}) = F_l^{-1}(\mathbf{v}) F_m^{-1}(\mathbf{v}) \left[\hat{f}_l \hat{f}_m \hat{B}(\mathbf{l},\mathbf{m})\right], \tag{2.6}$$

$$q^-(f)(\mathbf{v}) = F_m^{-1}(\mathbf{v}) \left[\hat{f}_m \hat{B}(\mathbf{m},\mathbf{m})\right], \tag{2.7}$$

where

$$\hat{B}(\mathbf{l},\mathbf{m}) = \int_{\mathbb{R}^3}\int_{S^2} B(|\mathbf{u}|,\theta) e^{2\pi\imath(\frac{\mathbf{l}+\mathbf{m}}{2},\mathbf{u})} e^{2\pi\imath|\mathbf{u}|(\frac{\mathbf{m}-\mathbf{l}}{2},\omega)}\, d\omega d\mathbf{u}. \tag{2.8}$$

The gain term is a kind of bilinear pseudodifferential operator with symbol $\hat{B}(\mathbf{l},\mathbf{m})$. The kernel $\hat{B}(\mathbf{l},\mathbf{m})$ is a distribution, hence for using it in practical

computations we have to regularize it. We will choose in a proper way the constant $R > 0$ and write the regularized kernel as

$$\hat{B}_R(\mathbf{l},\mathbf{m}) = \int_{\mathcal{B}(0,R)} \int_{S^2} B(|\mathbf{u}|,\theta) e^{2\pi\imath(\frac{\mathbf{l}+\mathbf{m}}{2},\mathbf{u})} e^{2\pi\imath|\mathbf{u}|(\frac{\mathbf{m}-\mathbf{l}}{2},\omega)}\, d\omega d\mathbf{u}. \tag{2.9}$$

We denote by $Q_R^+(f,f)$ and $q_R^-(f)$ the gain and collision frequency terms with regularized kernel $\hat{B}_R$.

The kernel $\hat{B}_R$ can be computed analytically for some special cases of VHS model (see [22]). In particular, for hard sphere gas it is given by

$$\hat{B}_R(\mathbf{l},\mathbf{m}) = \\ 8\frac{p^2\left[\pi Rq\sin(\pi Rq)+\cos(\pi Rq)\right] - q^2\left[\pi Rp\sin(\pi Rp)+\cos(\pi Rp)\right] - 4\xi\eta}{\pi^2\xi\eta p^2 q^2},$$

whereas for Maxwellian gas we have the following formula

$$\hat{B}_R(\mathbf{l},\mathbf{m}) = 2\frac{p\sin(\pi Rq) - q\sin(\pi Rp)}{\pi^2\xi\eta pq},$$

where $p = \xi + \eta$, $q = \xi - \eta$ and $\xi = |\mathbf{l}+\mathbf{m}|$, $\eta = |\mathbf{l}-\mathbf{m}|$.

3. Discretization of the collision integral

3.1. **Discretization of velocity space.** We will illustrate our approach to the numerical solution of the Boltzmann equation by space homogeneous problems with discontinuous initial data. A standard semi-implicit finite difference scheme in time will be applied pointwise with respect to velocity variable.

The distribution function $f(t,\mathbf{v})$ is usually negligible small outside some ball, so for the numerical treatment of the Boltzmann equation we assume that

$$\text{supp } f \subset \Omega_v := [-L,L]^3,$$

where we take $L = \frac{1}{2}$ for the technical reason which will be given later.

One of the main problems with efficient deterministic computation of the Boltzmann equation is a fixed usually uniform discretization of the velocity domain. Hence a huge number of discretization points is required to get the desired accuracy.

We overcome this problem by introducing a nonuniform velocity grid $\mathcal{G}_v \subset \Omega_v$ with N_v denoting the number of points in $\mathcal{G}_v$. The grid $\mathcal{G}_v \subset \Omega_v$ of discrete points will be chosen in such a way that the jump of the function values between neighboring points is lower than some prescribed threshold. Thus the grid will have much more discrete points in regions where the function changes rapidly than in the regions where the function is almost constant. In

order to treat the discontinuous functions we impose an additional condition that the neighboring points should not be closer than some given number.

The numerical method that we introduce in this paper gives a possibility after some preprocessing to compute approximate values of the gain term $Q^+(f,f)$ and the collision frequency $q^-(f)$ at arbitrary points in velocity space for a very low cost. It makes that $Q_R^+(f,f)$ and $q_R^-(f)$ can be computed effectively on a non-uniform grid different from one where the function f is defined.

This property lets to a natural idea to built at each time step a nonuniform grid in Ω_v that is changed adaptively to follow the the changes of the distribution function f (see Section 4).

At each time step we will first compute the values of the solution at vertexes of cells that build some initial coarse grid. Then using some reasonable criteria we will decide which cells in this coarse grid must be divided into smaller ones. The simplest criteria is a threshold for the variation of the solution within the cell.

After dividing chosen cells we compute values of the solution in new vertexes of the new cells and then continue the subdivision in the same way. Thus we generate much more grid points in parts of Ω_v where the function f changes rapidly than in those where the function is almost constant. In order to treat discontinuous functions we impose an additional condition that the neighboring points should not be closer than some given number.

During this process of subdivision we create an adaptive grid in parallel with computation of the values of the solution at each time step. Details of this adaptive procedure like distribution of grid points and the shape of the cells can be managed in various ways. They are in our method completely independent from the main challenge that is the effective computation of the gain term $Q_R^+(f,f)$ on an arbitrary non-uniform grid.

Particular adaptive grids that we use in examples at the end of the paper are grids consisting of an hierarchy of cubes, subdivided into eight smaller ones in a binary way in regions with high variation of f.

3.2. **Discretization of Fourier transform.** Now we focus on the numerical approximation of the Fourier transform integrals (2.4) and (2.5) for f defined on a non-regular grid.

We have restricted the function f to a bounded domain Ω_v. See [22] for discussion of the validity of such a restriction. For the sake of simplicity we will describe here the evaluation of the integral

$$\hat{f}_m = \int_{\Omega_v} f(\mathbf{v}) e^{2\pi i(\mathbf{v},\mathbf{m})}\, d\mathbf{v},$$

for f approximated by a function $\bar{f}$ piecewise constant on cells defined by the discretization of the velocity space. The approach we use below does not depend on this issue.

Using an approximation $\bar{f}$ for f we get the following discrete in velocity variable approximation for Fourier transform of f (we keep the same notation for the Fourier transform and its discretization)

$$\hat{f}_m = \sum_K \bar{f}_K \int_K e^{2\pi\imath(\mathbf{v},\mathbf{m})}\, d\mathbf{v} = \sum_K C_m \bar{f}_K \sum_{\mathbf{v}_K} e^{2\pi\imath(\mathbf{v}_K,\mathbf{m})},$$

where K denotes a cubic cell of the discretization of Ω_v, $\bar{f}_K$ is a constant approximating f on K and C_m is a constant depending only on $\mathbf{m}$. The above formulation has a disadvantage that some points are counted multiple times depending on how many cells have the given point in common. To avoid this multiple counting we build the *unique-node* grid of velocity points to get the following formulation

$$\hat{f}_m = C_m \sum_j \bar{f}_j\, e^{2\pi\imath(\mathbf{v}_j,\mathbf{m})}, \tag{3.1}$$

where $\bar{f}_j$ is a value of function f in a point $\mathbf{v}_j$. Another higher order approximation for f on cells using values $\bar{f}_j$ in vertexes of the cells would lead to a similar formula.

The standard Fast Fourier Transform (FFT) algorithm commonly used to compute numerically trigonometric sums cannot be used here for sums like one in (3.1), since the points $\mathbf{v}_j$ in the velocity space Ω_v are not equidistant. To manage this problem we use the *Unequally Spaced Fast Fourier Transform* (USFFT) algorithm developed by G. Beylkin [4]. This procedure is convenient to formulate if we scale the problem so that points $\mathbf{v}_j$ lay within the cube $[-\frac{1}{2},\frac{1}{2}]^3$. Hence we assume later that the problem is scaled so that the support of the function f lies in such a cube.

Below we give for completeness of the presentation an outline of the algorithm. Values of Fourier transform $\hat{f}_m$ by formula (3.1) will be computed on a uniform grid in R^3 in Fourier domain: $\{\mathbf{m} = (m_1, m_2, m_3) : m_1, m_2, m_3 = -M, \ldots, M-1\}$ for $M = 2^{-n-2}$ with $n < 0$. We will use for brevity the shortened notation $\mathbf{m} = -M, \ldots, M-1$ for multi-indices denoting points of such grids. Hence we need to compute the sum (3.1) for $\mathbf{m} = -M, \ldots, M-1$.

Let $N = 4M$. The first step is computing the coefficients

$$g_k = \sum_j \bar{f}_j \beta^{(p)}_{k_1,n}(v_{j,1}) \beta^{(p)}_{k_2,n}(v_{j,2}) \beta^{(p)}_{k_3,n}(v_{j,3}), \quad \mathbf{k} = 0, \ldots, N-1,$$

where $\mathbf{v}_j = (v_{j,1}, v_{j,2}, v_{j,3})$ and $\beta^{(p)}_{r,n}(x) = 2^{-\frac{n}{2}} \beta^{(p)}(2^{-n}x - r)$ with $\beta^{(p)}$ being the central B-spline of order p. The computational cost of this step is $\mathrm{O}(p^3 N_v)$.

Then we evaluate a trigonometric sum

$$F_l = \sum_{\mathbf{k}=0}^{N-1} g_k e^{2\pi\imath(\mathbf{k},\mathbf{l})/N}, \quad \mathbf{l} = -N/2, \ldots, N/2-1$$

using standard FFT algorithm with the cost $\mathrm{O}(N^3 \log N)$.

The last step is a scaling of Fourier transform F_l according to the formula

$$\hat{f}_m = \frac{1}{N^{\frac{3}{2}}\sqrt{a^{(p)}(m_1/N)a^{(p)}(m_2/N)a^{(p)}(m_3/N)}} F_m, \quad \mathbf{m} = -M, \ldots, M-1.$$

This step requires only $\mathrm{O}(N^3)$ multiplications, hence the total cost of the USFFT algorithm can be estimated as $\mathrm{O}(p^3 N_v)+\mathrm{O}(N^3 \log N)$. The precision of these computations depends on the order p of the the central B-splines $\beta^{(p)}$ and on the oversampling that is relation between 2 in this case.

A similar procedure is used to calculate the inverse Fourier transform (2.5) which, discretized in Fourier domain, is given by

$$f(\mathbf{v}) = \sum_{\mathbf{m}=-M}^{M-1} \hat{f}_m e^{-2\pi\imath(\mathbf{m},\mathbf{v})}, \quad \mathbf{v} \in \Omega_v. \tag{3.2}$$

Namely, we start with extending the Fourier coefficients

$$g_k = \begin{cases} \hat{f}_{k+M} & \text{if } -M \le \mathbf{k} \le M-1, \\ 0 & \text{otherwise,} \end{cases} \qquad \mathbf{k} = -N/2, \ldots, N/2-1.$$

Then we scale g_k according to the formula

$$\tilde{g}_k = \frac{g_k}{\hat{b}_{k_1}\hat{b}_{k_2}\hat{b}_{k_3}},$$

where $\hat{b}_{k_j} = \sum_{l=-\frac{p-1}{2}}^{\frac{p-1}{2}} \beta^{(p)}(l) e^{2\pi\imath l k_j/N}$. Next we apply the FFT algorithm to compute the sum

$$f_l = \sum_{\mathbf{k}=-N/2}^{N/2-1} \tilde{g}_k e^{2\pi\imath(\mathbf{l},\mathbf{k})/N}, \quad \mathbf{l} = -N/2, \ldots, N/2-1.$$

Finally, we evaluate f at any point $\mathbf{v} \in \Omega_v$ using the formula

$$f(\mathbf{v}) = \sum_{\mathbf{l}=-N/2}^{N/2-1} f_l \beta^{(p)}(\frac{N}{2}v_1 - l_1)\beta^{(p)}(\frac{N}{2}v_2 - l_2)\beta^{(p)}(\frac{N}{2}v_3 - l_3).$$

The cost of the first two steps of the algorithm is $\mathrm{O}(N^3 \log N)$. The cost of the last step depends on the number of required computations of f in the velocity domain and for N_v points it is $\mathrm{O}(p^3 N_v)$. Hence the total cost of calculation of the inverse Fourier transform is the same as before.

3.3. **Decomposition of the gain term $Q^+(f,f)$.** Discretization of the collision operator is splitted into two parts according to (2.1). We start with the gain term $Q^+(f,f)$ (2.2), which is discretized as follows

$$Q^+(f,f)(\mathbf{v}) = \sum_{\mathbf{l},\mathbf{m}=-M}^{M-1} \hat{f}_l \hat{f}_m \hat{B}(\mathbf{l},\mathbf{m}) e^{-2\pi\imath(\mathbf{l}+\mathbf{m},\mathbf{v})}.$$

To reduce the computational cost of this formulation we want to decouple dependence on variables $\mathbf{l}$ and $\mathbf{m}$ in the kernel $\hat{B}(\mathbf{l},\mathbf{m})$. This makes the bilinear expression easy to calculate.

It is easy to check that the kernel $\hat{B}(\mathbf{l},\mathbf{m})$ is a symmetric matrix. It is a function of $|\mathbf{l}-\mathbf{m}|$, $|\mathbf{l}+\mathbf{m}|$ and $(\mathbf{l}-\mathbf{m})(\mathbf{l}+\mathbf{m})$ (and in the case of VHS model of $|\mathbf{l}-\mathbf{m}|$ and $|\mathbf{l}+\mathbf{m}|$ only) [22]. Hence we use the spectral decomposition to get

$$\hat{B}(\mathbf{l},\mathbf{m}) = \sum_{r=1}^{s} d_r U_r(\mathbf{l}) U_r(\mathbf{m}), \tag{3.3}$$

where $s = 8M^3$ is the number of eigenvalues and U_r is the eigenvector corresponding to the eigenvalue d_r. Obviously we can take in (3.3) only significant eigenvalues (with some prescribed threshold) to get a reasonable approximation of the kernel.

Now let s denote the number of significant eigenvalues of $\hat{B}(\mathbf{l},\mathbf{m})$, which is typically $\frac{1}{8}$ to $\frac{1}{4}$ part of the total number. Hence we get the following approximation to the gain term

$$Q^+(f,f)(\mathbf{v}) = \sum_{p=1}^{s} d_r \left[\sum_{\mathbf{m}=-M}^{M-1} \hat{f}_m U_r(\mathbf{m}) e^{-2\pi\imath(\mathbf{m},\mathbf{v})} \right]^2. \tag{3.4}$$

In our algorithm we need to compute the sum (3.4) in many arbitrary points $\mathbf{v}$ in the velocity domain Ω_v so that finally they will build an adaptive grid that suites well for the approximation of the solution f at the next time step. A straightforward calculation of the sum of squares in (3.4) would be too much time and memory consuming. To do it efficiently we compute first the sums $\sum_{\mathbf{m}=-M}^{M-1} \hat{f}_m U_r(\mathbf{m}) e^{-2\pi\imath(\mathbf{m},\mathbf{v})}$ on a regular grid in Ω_v using standard FFT algorithm and then compute (3.4) on the same regular grid. After that we compute the FFT of (3.4) back into the Fourier domain. Then the computation of $Q^+(f,f)(\mathbf{v})$ on an adaptive grid is done effectively by the USFFT algorithm described before.

The discretization of the loss term $Q^-(f,f)$ (2.3) consists of computation of the discrete collision frequency term (2.7)

$$q^-(f)(\mathbf{v}) = \sum_{\mathbf{m}=-M}^{M-1} \hat{f_m} \hat{B}(\mathbf{m},\mathbf{m}) e^{-2\pi\imath(\mathbf{m},\mathbf{v})},$$

which is a convolution operator and a pointwise multiplication of $q^-(f)(\mathbf{v})$ by $f(\mathbf{v})$. We compute $q^-(f)(\mathbf{v})$ again using USFFT algorithm with $\mathrm{O}(p^3 N_v) + \mathrm{O}(\sigma N^3 \log N)$ operations.

The total computational cost of the numerical approximation of the collision operator is $\mathrm{O}(p^3 N_v) + \mathrm{O}(\sigma N^6 \log N)$, where σ is a small number depending on the required accuracy in the approximation of the kernel $\hat{B}(\mathbf{l}, \mathbf{m})$.

We point out that the computational cost consists of two parts. The first one depends on the approximation of the discontinuous solution and increases linearly with the number N_v of points in the adaptive velocity grid. Another part depends on the approximation of the smooth terms in the equation. Here N is the number of Fourier modes along one coordinate direction necessary for approximating smooth terms in the Boltzmann equation that is moderate, It implies that the suggested deterministic method for computing the Boltzmann collision operator seems to be considerably more effective than previous ones.

4. Time discretization

The homogeneous Boltzmann equation is solved numerically using the standard semi-implicit Euler scheme

$$\frac{f^{n+1} - f^n}{\Delta t} = Q^+(f^n, f^n) - f^{n+1} q^-(f^n),$$

where $f^n = f(t_n)$ denotes the solution f at time t_n. Solving this equation for f^{n+1} we get

$$f^{n+1} = \frac{f^n + \Delta t\, Q^+(f^n, f^n)}{1 + \Delta t\, q^-(f^n)}. \tag{4.1}$$

A higher order finite difference scheme can be also easily adapted.

4.1. Conservation procedure.

Since the Boltzmann equation is based on a balance principle and since the hydrodynamic equations for the macroscopic quantities have the form of the conservation laws, one may expect that the proper numerical scheme should in some sense reflect these properties. However the proposed numerical scheme, as a spectral method do not representing higher moments of solutions exactly, conserves only mass – momentum and energy are not conserved.

A correction technique which enforces the conservativeness was proposed by Aristov and Tcheremisin (see [2]). The numerical solution f^{n+1} given by (4.1) is corrected by adding a term

$$f^{n+1} \sum_{i=0}^{4} \alpha_i \psi_i,$$

where $\psi_0(\mathbf{v}) = 1$, $\psi_i(\mathbf{v}) = v_i$ for $i = 1, 2, 3$, and $\psi_4(\mathbf{v}) = |\mathbf{v}|$. The numbers α_i are determined by requiring that the (discretized) conservation laws

$$\sum_{\mathbf{v}_j \in \mathcal{G}_v} \psi_l(\mathbf{v}_j) f^{n+1}(\mathbf{v}_j) \Big(1 + \sum_{i=0}^{4} \alpha_i \psi_i(\mathbf{v}_j)\Big) = \sum_{\mathbf{v}_j \in \mathcal{G}_v} \psi_l(\mathbf{v}_j) f^n(\mathbf{v}_j)$$

are satisfied for $l = 0, \ldots, 4$.

Hence we get the following formula for the solution

$$f^{n+1} = \frac{f^n + \Delta t\, Q^+(f^n, f^n)}{1 + \Delta t\, q^-(f^n)} \Big(1 + \sum_{i=0}^{4} \alpha_i \psi_i\Big). \tag{4.2}$$

4.2. **Adaptive grid.** At each time step a new grid (based on existing one) is built for the solution f^{n+1} according to the formula (4.2).

We build this grid using the values of f^n on the existing grid. In case the grid should be finer (we need more nodes in the new grid) we interpolate the values of f^n on the neighboring nodes. We use for this purpose a simple trilinear interpolation i.e. the interpolating function is linear in each direction. The values of $Q^+(f^n, f^n)$ and $q^-(f^n)$ are computed straightforwardly at the desired points using the inverse USFFT algorithm.

5. Numerical examples

We illustrate our new method on several examples with discontinuous initial data. Having in mind future applications of our approach to boundary value problems we chosen data with discontinuities typical for flows around bodies. Despite the simplicity of these examples they reflect certain computational problems one is faced with solving boundary value problems.

If we think about the flow around a body then simple physical reasons based on the collisionless picture of gas dynamics imply that the distribution function $f(t, x, v)$ at a space point x should include two type of inputs. These are the input from the particles coming from the body and having corresponding temperature and zero mean velocity. Another one is the input from the particles coming from infinity and having large mean velocity and another temperature. Depending on the position of the point x with respect the body and depending on the shape of the body one observes different cone like surfaces of discontinuity in the distribution function.

We present here numerical results for maxwell molecules. On the other hand our method is independent of this particular model.

Example 1.

The first example is the evolution starting from the initial distribution function $f_0(v)$ that is a maxwell distribution function with temperature 0.0115 and velocity 0 in the half space $x \leq 0$ and is another maxwell distribution with temperature 0.0115 and velocity -0.1 in the half space $x < 0$

. Therefore f_0 is discontinuous on the $y - z$ plane. This function imitates the distribution of the gas close to the surface of a body with the similar temperature.

Example 2. The second example imitates the distribution function in the gas flow around a sphere at a point x at some finite distance from the sphere. We chosen the initial distribution $f_0(\mathbf{v})$ similar to one that is observed in such a flow if collisions between molecules are absent. Namely the distribution function is initially equal to a maxwell distribution function with temperature 0.0115 and velocity 0 for points within a cone with center at the origin. This part of the distribution function imitates particles reflected from the body. Outside of this cone the initial distribution function is taken equal to another maxwell distribution with temperature 0.0065 and velocity -0.1. This part of the distribution functions imitates the flow coming from infinity. Therefore in this case the initial distribution has a discontinuity at the surface of a cone. We have chosen a cone having the axis laying in x-z plane with angle 135^0 with respect to x- axis. The cosine of the angle between the cone and its axis is 0.85.

Example 3.

The third example is given to illustrate the flexibility of the method to solutions with large difference of gradients. The initial data is similar to one in the first example but maxwell distributions in two half spaces have different temperatures 0.0115 and 0.065 and there are no particles within a gap in velocities with $-0.1 < v_x < 0$.

For each of these examples we present a sequence of graphs for values of the distribution function $f(t_i, \mathbf{v})$ for several time points $t_i = 0.02 * i$. in x-z plane and also the corresponding crossections of the three dimensional adaptive grid with x-z plane.

One can see in all these numerical results that the initial discontinuity in the distribution function decreases but preserves its position in complete accordance with known properties of the Boltzmann equation.

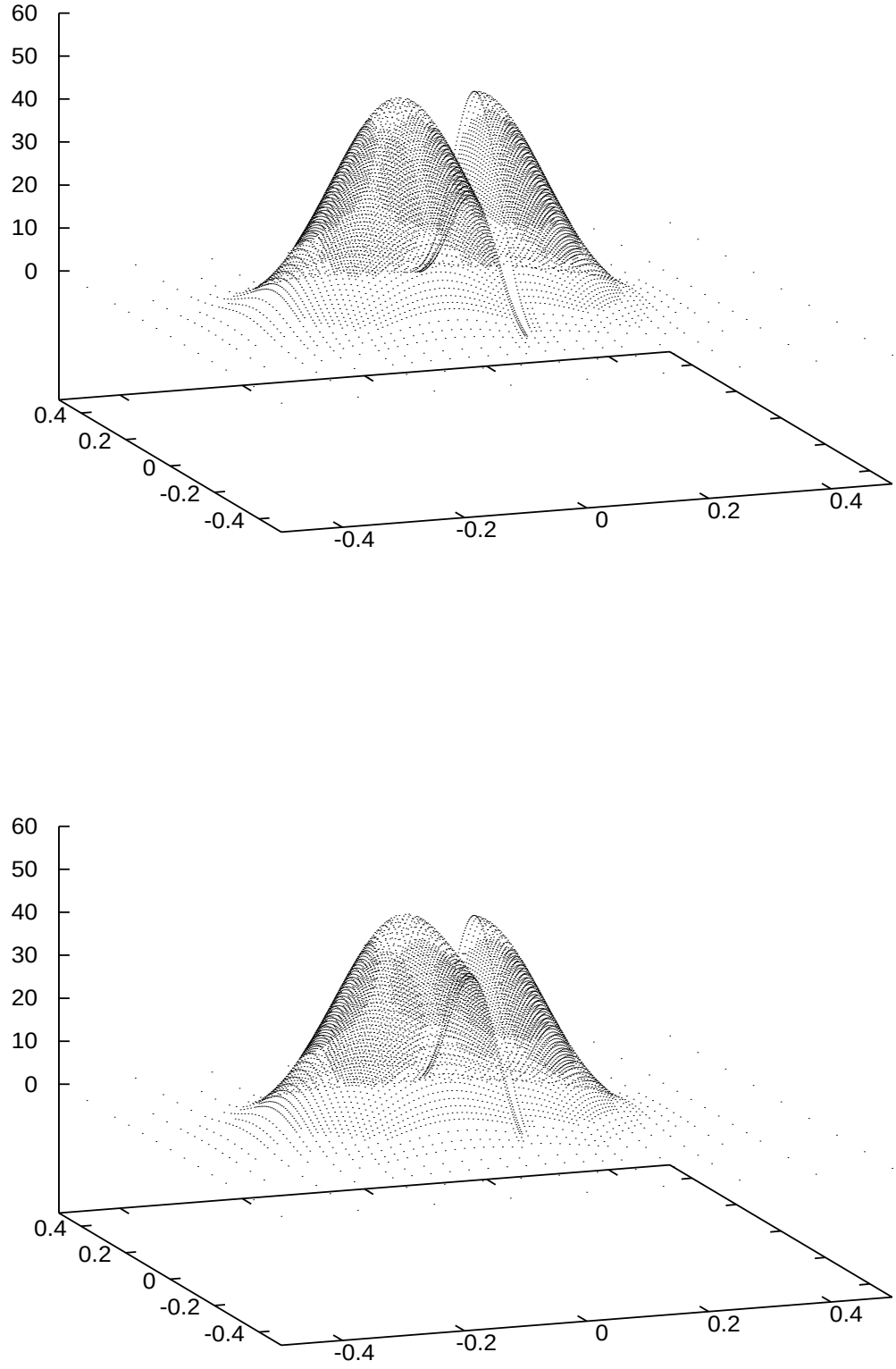

FIGURE 2. Example 1, solution steps 0 and 5

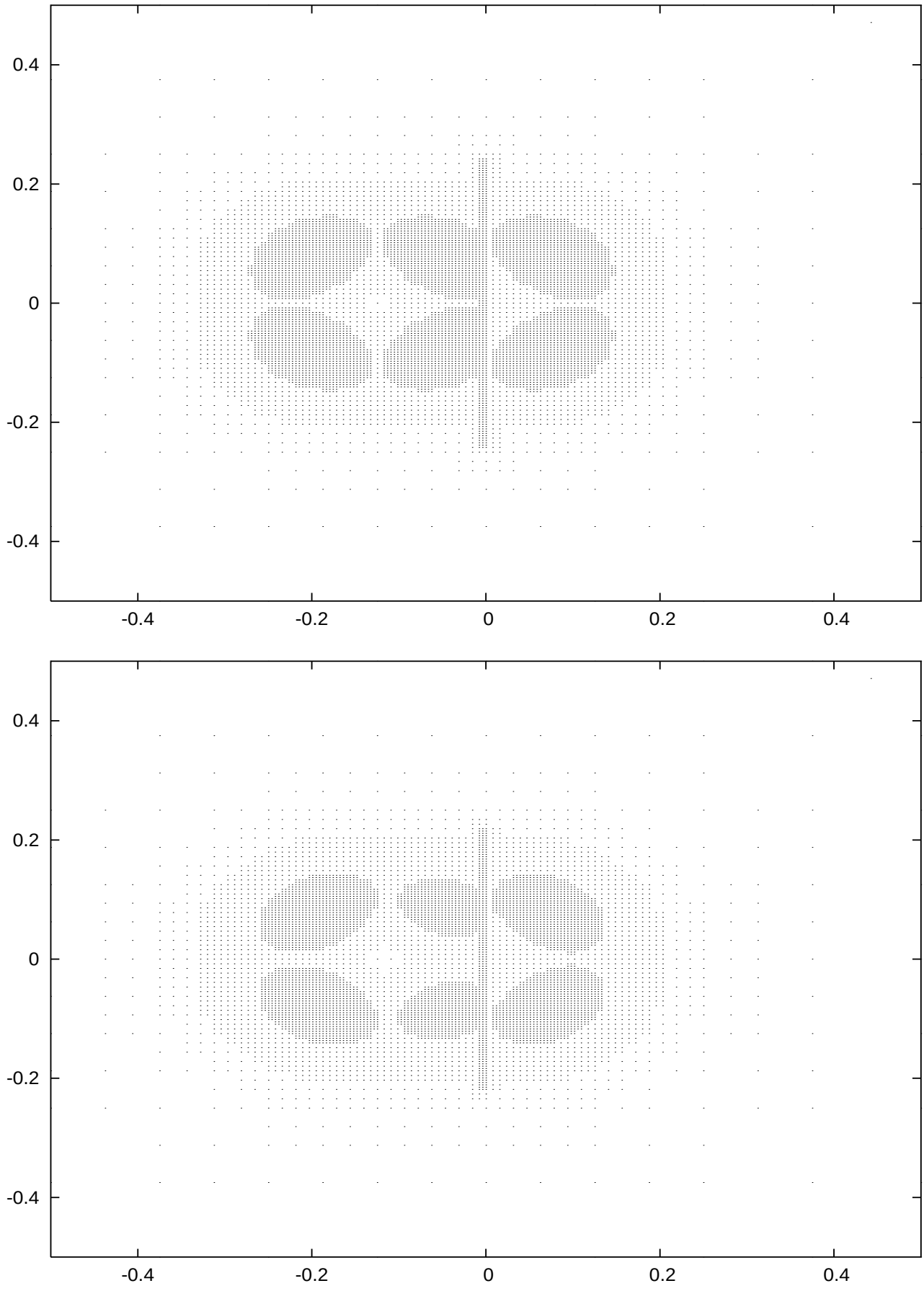

FIGURE 3. Example 1, grid steps 0 and 5

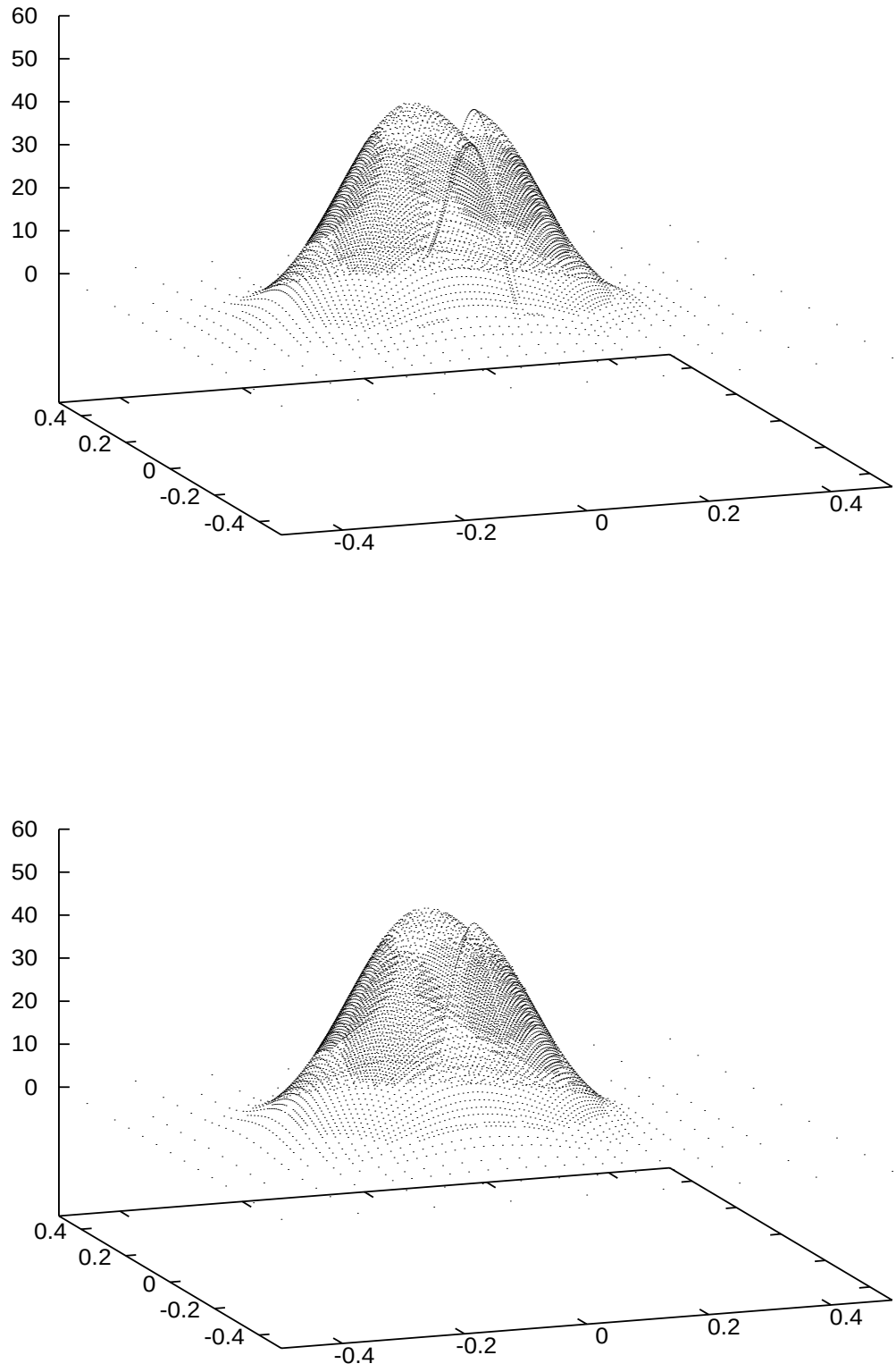

FIGURE 4. Example 1, solution steps 40 and 80

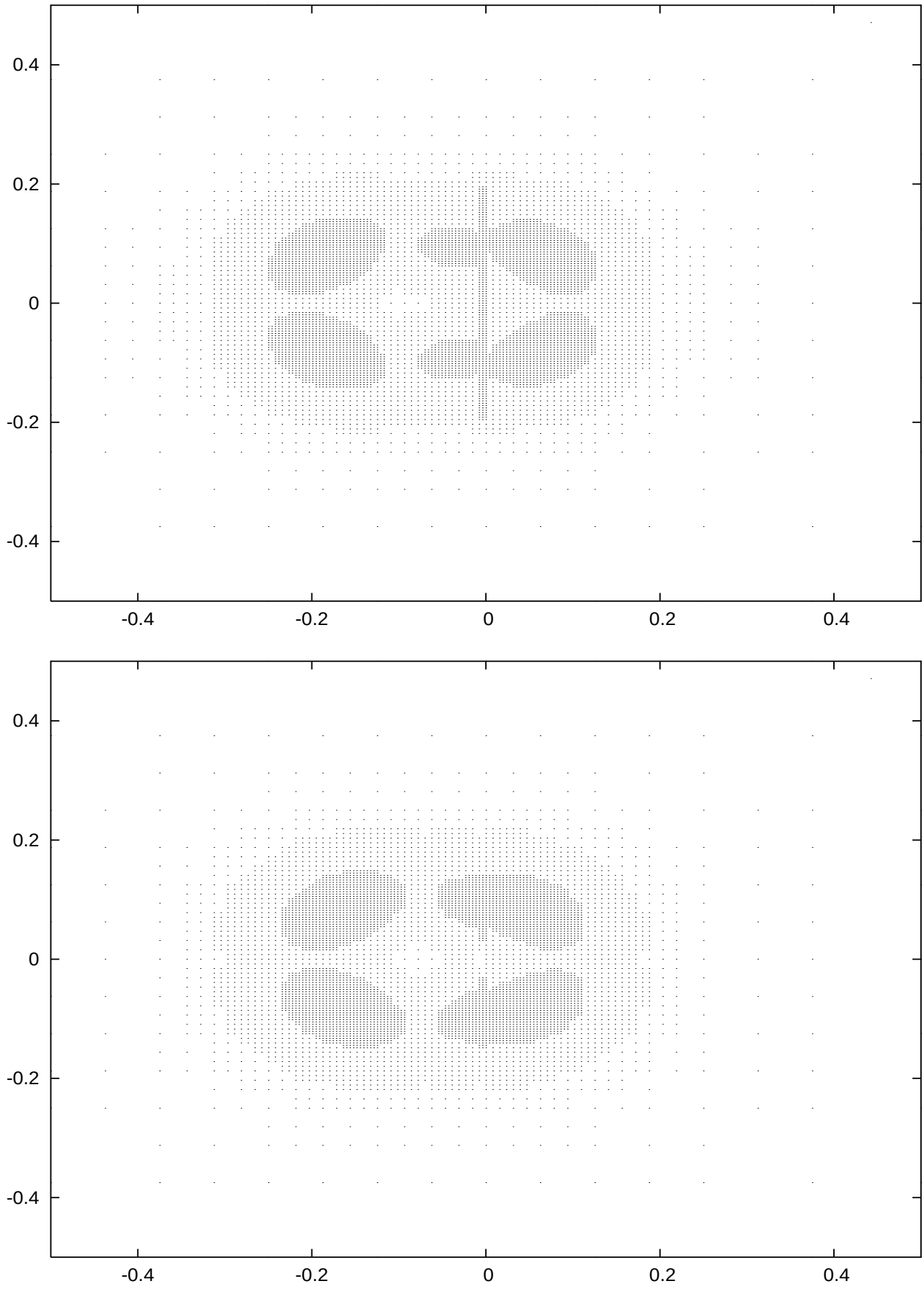

FIGURE 5. Example 1, grid steps 40 and 80

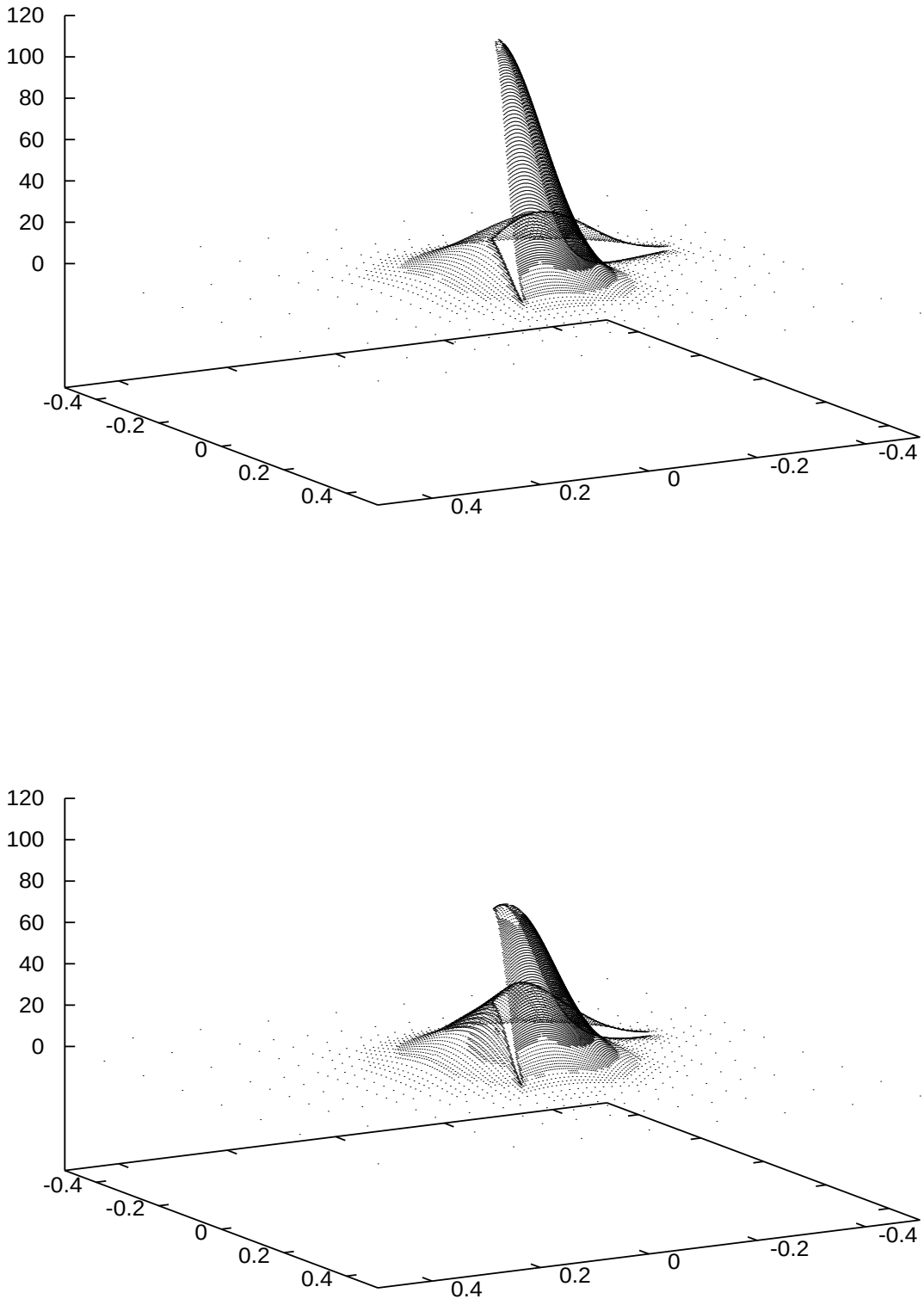

FIGURE 6. Example 2 solution steps 0 and 10

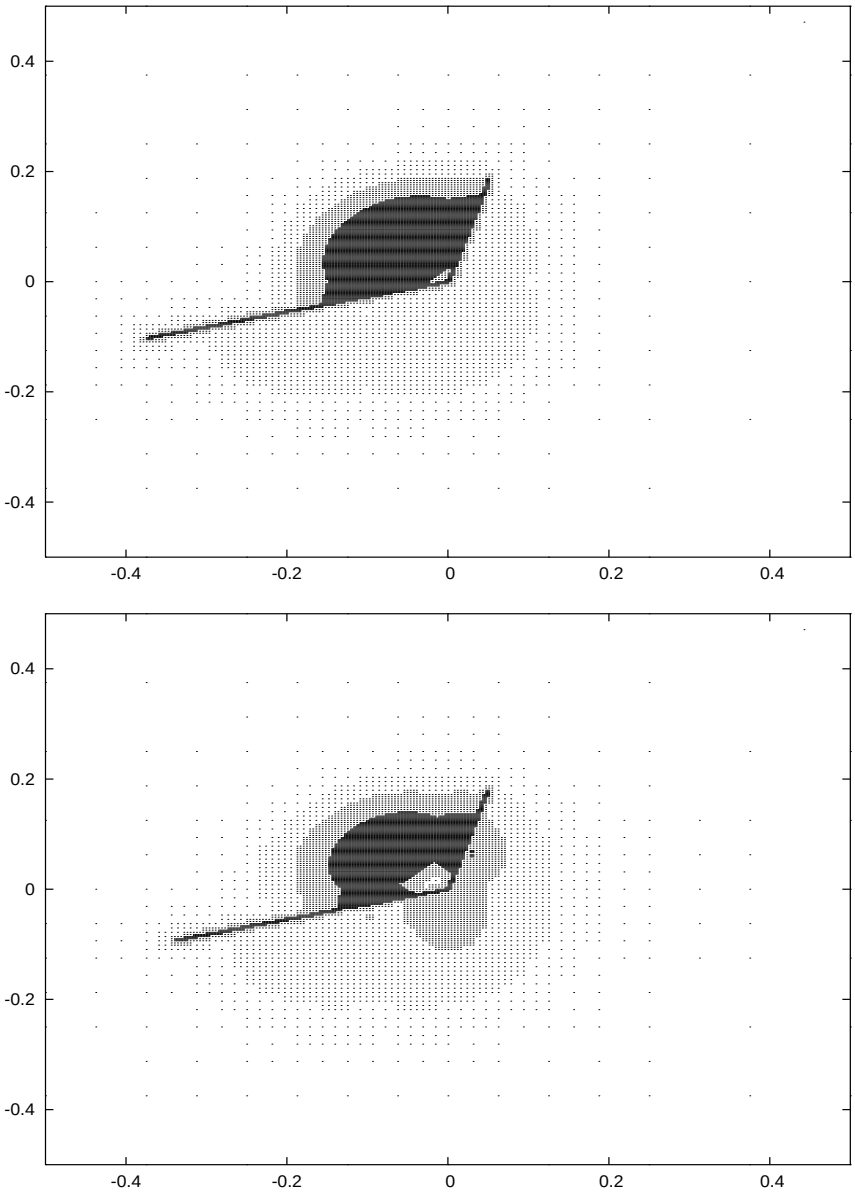

FIGURE 7. Example 2, grid steps 0 and 10

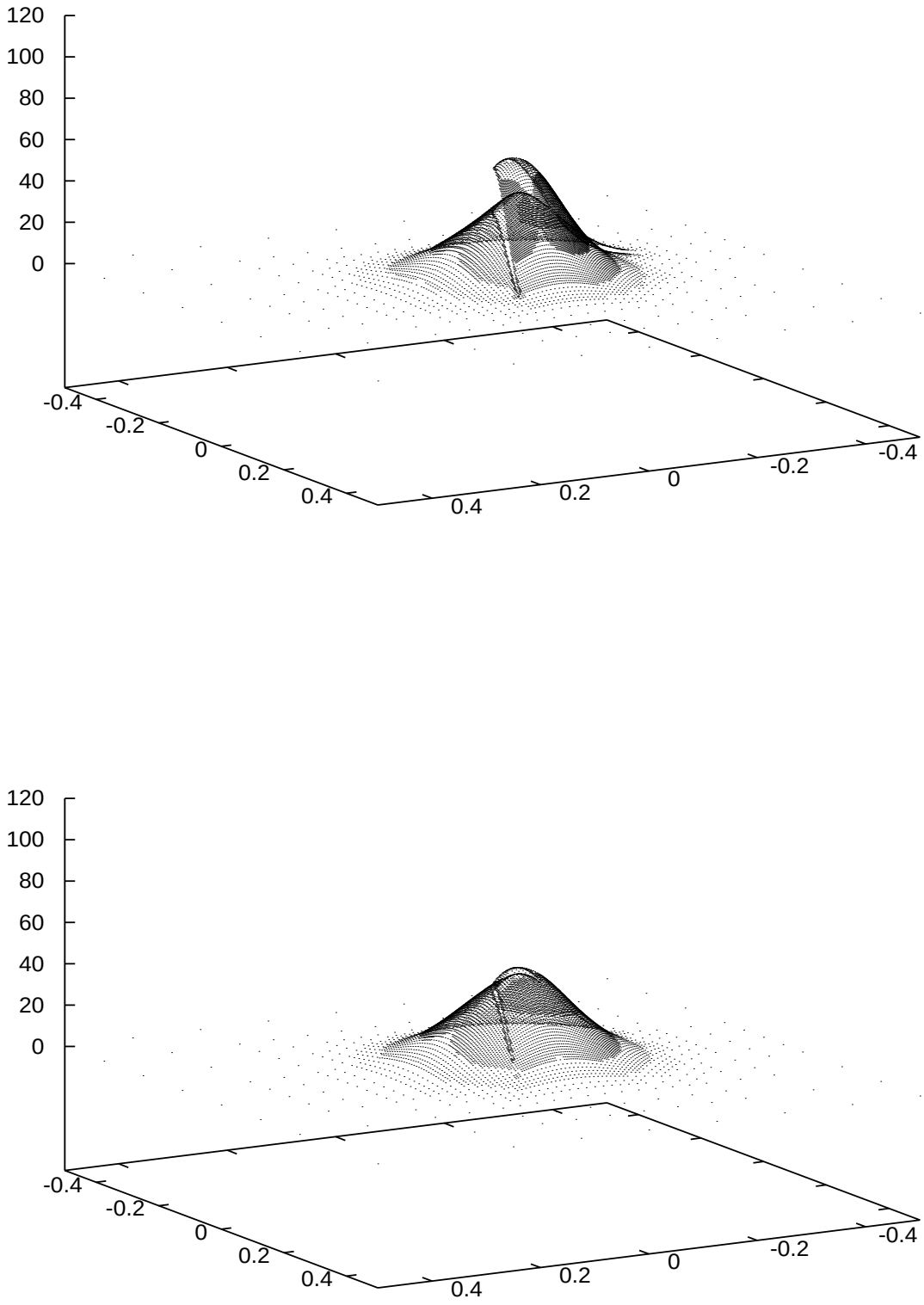

FIGURE 8. Example 2, solution steps 20 and 40

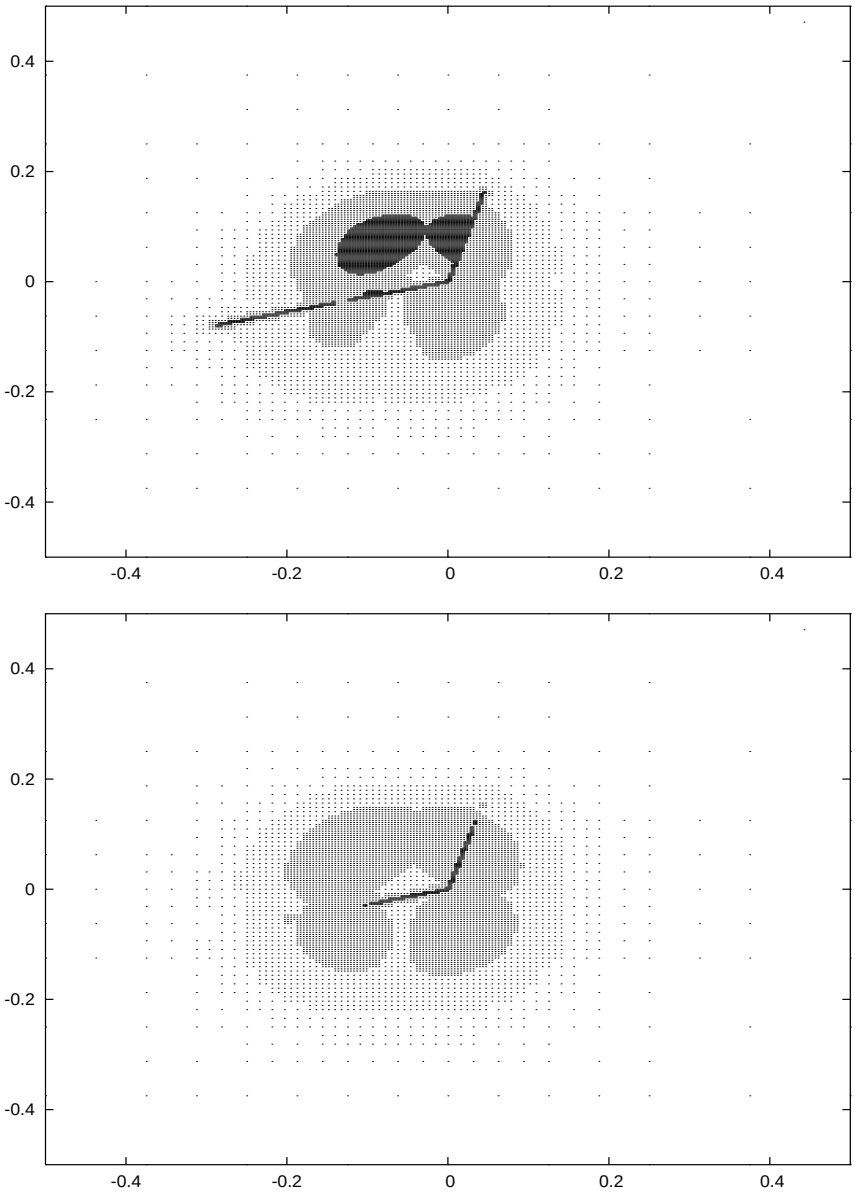

FIGURE 9. Example 2, grid steps 20 and 40

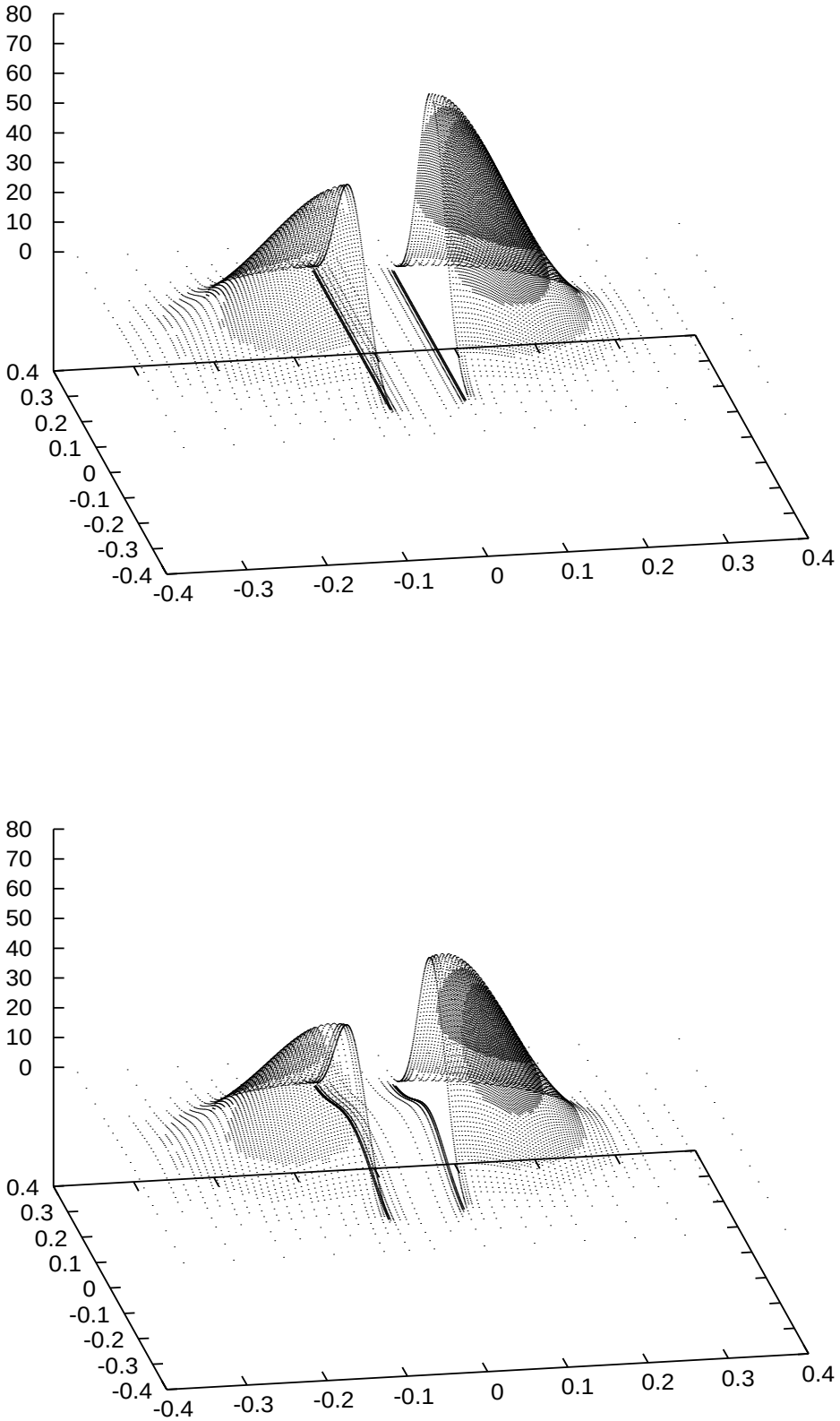

FIGURE 10. Example 3, solution steps 0 and 5

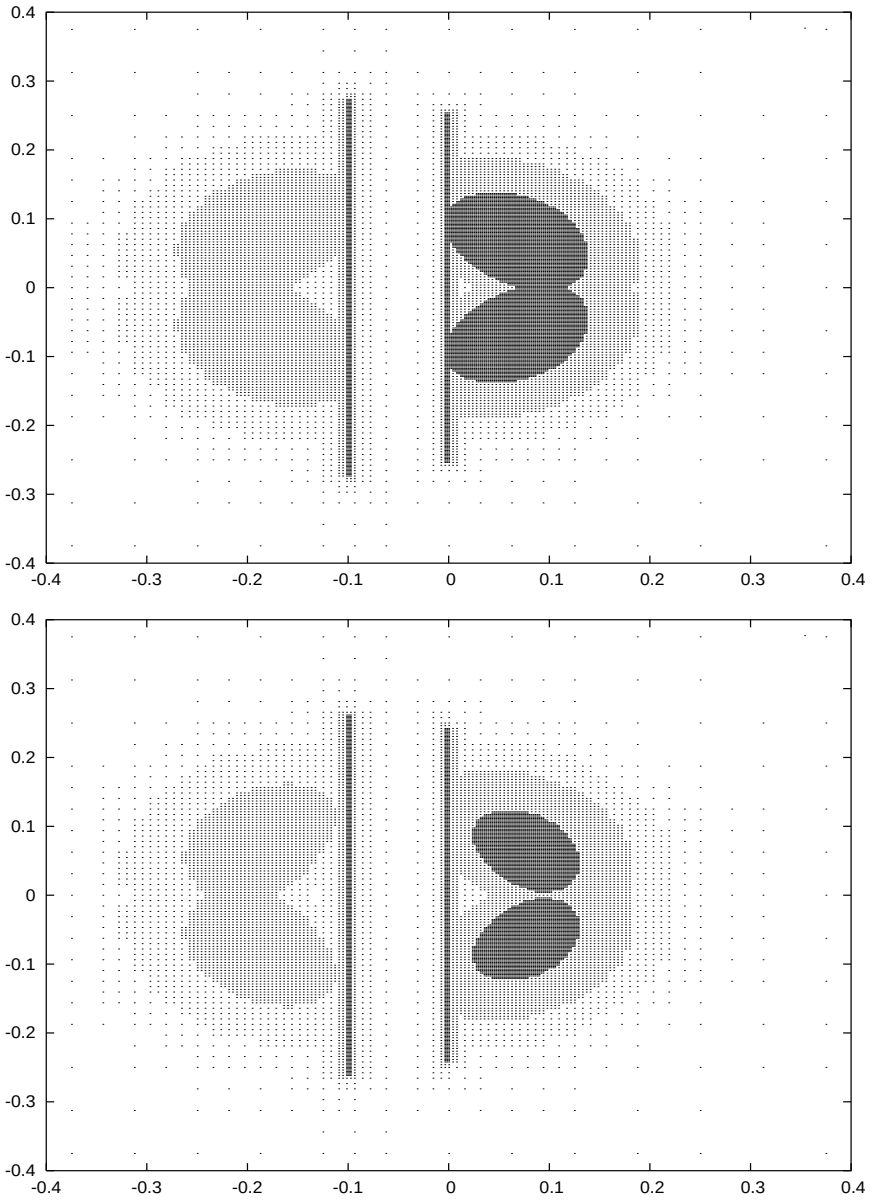

FIGURE 11. Example 3, grid steps 0 and 5

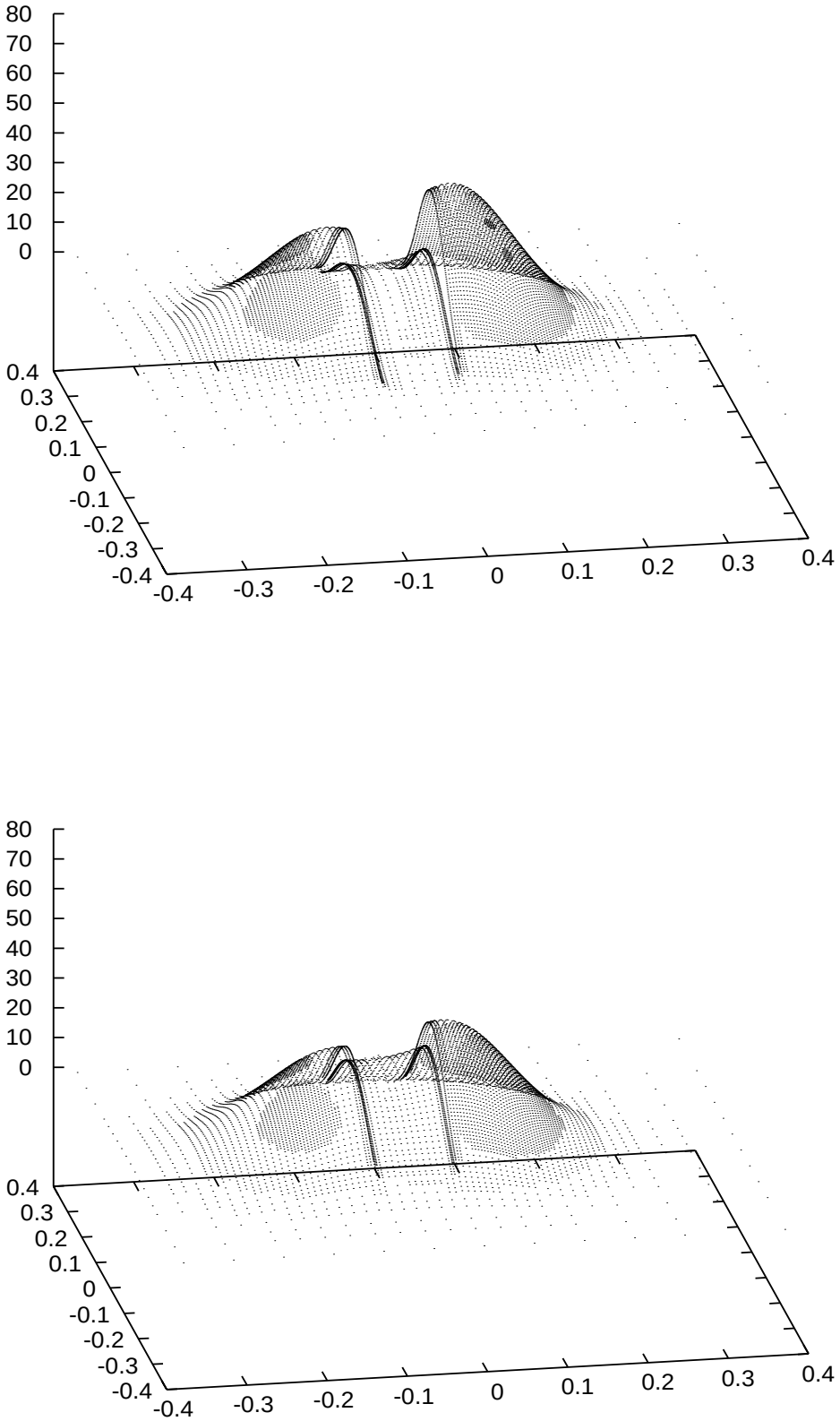

FIGURE 12. Example 3, solution steps 15 and 25

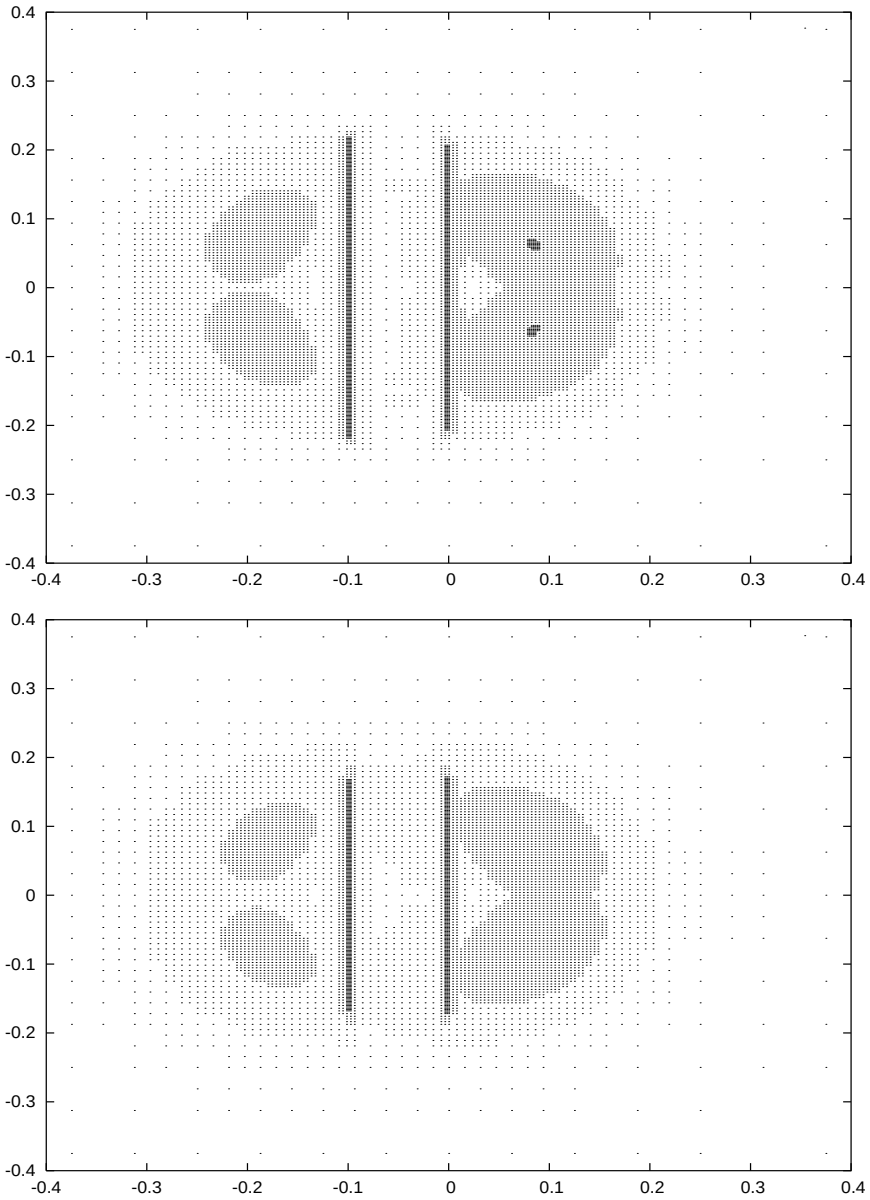

FIGURE 13. Example 3, grid steps 15 and 25

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