HAL
open science

Local discrete velocity grids for deterministic rarefied flow simulations

Stéphane Brull, Luc Mieussens

▶ **To cite this version:**

Stéphane Brull, Luc Mieussens. Local discrete velocity grids for deterministic rarefied flow simulations. Journal of Computational Physics, 2014, 266 (1), pp.22-46. 10.1016/j.jcp.2014.01.050 . hal-00808613v3

HAL Id: hal-00808613

https://hal.science/hal-00808613v3

Submitted on 14 Mar 2014

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Local discrete velocity grids for deterministic rarefied flow simulations

S. Brull[1], L. Mieussens[2]

[1]Univ. Bordeaux, IMB, UMR 5251, F-33400 Talence, France.
CNRS, IMB, UMR 5251, F-33400 Talence, France.
(Stephane.Brull@math.u-bordeaux1.fr)

[2]Univ. Bordeaux, IMB, UMR 5251, F-33400 Talence, France.
CNRS, IMB, UMR 5251, F-33400 Talence, France.
INRIA, F-33400 Talence, France.
(Luc.Mieussens@math.u-bordeaux1.fr)

Abstract

Most of numerical methods for deterministic simulations of rarefied gas flows use the discrete velocity (or discrete ordinate) approximation. In this approach, the kinetic equation is approximated with a global velocity grid. The grid must be large and fine enough to capture all the distribution functions, which is very expensive for high speed flows (like in hypersonic aerodynamics). In this article, we propose to use instead different velocity grids that are local in time and space: these grids dynamically adapt to the width of the distribution functions. The advantages and drawbacks of the method are illustrated in several 1D test cases.

Keywords: kinetic equations, discrete velocity model, deterministic method, rarefied gas dynamics

1 Introduction

Most of deterministic numerical methods for rarefied flow simulations are based on a discrete velocity approximation of the Boltzmann equation, see for instance [25, 23, 8, 7, 6, 19, 20, 16, 26, 14].

In almost all these methods, the distribution function is approximated with a global velocity grid, for every point in the position space, for every time. This makes the method robust (conservation, entropy dissipation, positivity, stability, etc.) and relatively simple, but very expensive for many cases. Indeed, the grid must be large enough to contain all the distribution functions of the flow, and fine enough to capture every narrow distributions. The first constraint makes the grid very large for high speed flow with large temperatures. The second constraint makes the grid step very small, and hence a very large number of discrete velocities are needed. This is for instance the case for atmospheric re-entry problems, where the flow is hypersonic. These problems, especially in 3D, are very difficult to be simulated

with such methods, due to the discrete velocity grid that contains a prohibitively large number of points.

Of course, particle solvers like the popular Direct Simulation Monte-Carlo method (DSMC) do not suffer of such problems [5]. However, if one is interested in deterministic Eulerian simulations, it is important to find a way to avoid the use of a too large number of discrete velocities. Up to our knowledge, there are a few papers on this subject. Aristov proposed in [1] an adaptive velocity grid for the 1D shock structure calculation. However, the approach is very specific to this test case and has never been extended. More recently, Filbet and Rey [12] proposed to use a rescaling of the velocity variable to make the support of the distribution independent of the temperature and of the macroscopic velocity. Then the Boltzmann equation is transformed into a different form (with inertia terms due to the change of referential). In [2], Baranger et al. proposed an algorithm to locally refine the velocity grid wherever it is necessary and to coarsen it elsewhere. But this approach, which has been proved to be very efficient for steady flows, is still based on a global grid, and cannot be efficient enough for unsteady flows. Finally, Chen et al. [9] proposed to use a different velocity grid for each point in the position space and every time: from one point to another one, the grid is refined or coarsen by using an Adaptive Mesh Refinement (AMR) technique. This seems to be very efficient, but all the grids have the same bounds (they all use the same background grid). It seems that a similar method was proposed at the same time by Kolobov et al., see [17, 15].

In this paper, we propose a method that has several common features with the method of [27] and [12] but is still very different. The main difference is that each distribution is discretized on its own velocity grid: each grid has its own bounds and step that are evolved in time and space by using the local macroscopic velocity and temperature. These macroscopic quantities are estimated by solving the local conservation laws of mass, momentum, and energy. The interaction between two space cells requires to use reconstruction techniques to approximate a distribution on different velocity grids. This paper is a preliminary work, for 1D flows, that proposes a complete algorithmic approach. Several test cases illustrate the properties of the method and show its efficiency.

The outline of the paper is the following. In section 2 is presented a simple 1D kinetic Bhatnagar-Gross-Krook (BGK) model and its standard discrete velocity approximation. In section 3, the local discrete velocity grid approach is described. The numerical tests are given in section 4.

2 A simple 1D kinetic model and its standard velocity discretization

We consider a one-dimensional gas described by the mass density of particles $f(t, x, v)$ that at time t have the position x and the velocity v (note that both position x and velocity v are scalar). The corresponding macroscopic quantities can be obtained by the moment vector $U(t, x) = \langle mf(t, x, .)\rangle$, where $m(v) = (1, v, \frac{1}{2}|v|^2)$ and $\langle\phi\rangle = \int_{\mathbb{R}} \phi(v)\, dv$ for any velocity

dependent function. This vector can be written component wise by $U = (\rho, \rho u, E)$, where ρ, ρu, and E are the mass, momentum, and energy densities. The temperature T of the gas is defined by relation $E = \frac{1}{2}\rho|u|^2 + \frac{1}{2}\rho RT$, where R is the gas constant.

The evolution of the gas is governed by the following BGK equation

$$\partial_t f + v\partial_x f = \frac{1}{\tau}(M(U) - f), \tag{1}$$

where $M(U)$ is the local Maxwellian distribution defined through the macroscopic quantities U of f by

$$M(U) = \frac{\rho}{\sqrt{2\pi RT}} \exp\big(-\frac{|v-u|^2}{2RT}\big), \tag{2}$$

and $\tau = CT^\omega/\rho$ is the relaxation time. The constant C and ω will be given in section 4 for each test case.

From this equation, it is easy to establish the so called conservation laws that describe the time evolution of the moment vector U:

$$\partial_t U + \partial_x \langle vmf \rangle = 0. \tag{3}$$

For the numerical approximation of equation (1), a popular method is the discrete ordinate–or discrete velocity–method. It consists in choosing a grid $\mathcal{V}$ of K points v_k, and then in replacing the kinetic equation (1) by the finite set of K equations

$$\partial_t f_k + v_k \partial_x f_k = \frac{1}{\tau}(M_k(U) - f_k) \tag{4}$$

where $f_k(t,x)$ is an approximation of $f(t,x,v_k)$ and $M_k(U)$ is an approximation of $M(U)(v_k)$. This approximation is the discrete Maxwellian whose parameters are such that it has the same discrete moments as the distribution f, as proposed in [18, 19]. This gives a conservative discrete velocity model.

In order to describe the solution correctly, the discrete velocity grid $\mathcal{V}$ must capture all the distribution functions, that is to say at any time t, and for every position x. This means that $\mathcal{V}$ must be large enough to capture distributions with large mean velocity or large temperature, and fine enough to capture distributions with small temperature. See an illustration of this problem in figure 1. In this figure, we show a 2D aerodynamical flow with three typical distributions functions (one in the upstream flow, one in the shock, and another one at the boundary). The corresponding velocity grid is shown in the same figure.

To construct such a grid, we start with a remark on the local Maxwellians. Since a Maxwellian centered on u and of temperature T decreases very fast for large v, it is very small outside any interval $[u - c\sqrt{RT}, u + c\sqrt{RT}]$ with c sufficiently large. A good choice for such an interval is obtained with $c = 3\sqrt{RT}$: as it is well know in statistics for the normal distribution, 99% of the particles described by the local Maxwellian have their velocity in this interval. For kinetic simulations, we generally take a slightly larger interval with $c = 4$. The corresponding interval $[u - 4\sqrt{RT}, u + 4\sqrt{RT}]$ is what we call the "support" of the

local Maxwellian and contains the "essential" information on the distribution. When a distribution is not too far from its corresponding local Maxwellian (which is true when the Knudsen number is not too small, away from shock and boundary layers), most of particles described by this distribution have their velocity localized in the support of the corresponding local Maxwellian. This is interesting, since this support can be analytically determined as a function of the macroscopic velocity and temperature, as it has been shown above.

Consequently, a first constraint for the global velocity grid is that its bounds v_{min} and v_{max} satisfy the following inequalities:

$$v_{min} \leq \min_{t,x}\big(u(t,x) - 4\sqrt{RT(t,x)}\big), \qquad v_{max} \geq \max_{t,x}\big(u(t,x) + 4\sqrt{RT(t,x)}\big), \tag{5}$$

so that all the distributions can be captured in the grid. Since it is reasonable to require that there are at least three points between the inflexion points of any Maxwellian, the step of the global grid should be such that

$$\Delta v \leq \min_{t,x} \sqrt{RT(t,x)}. \tag{6}$$

Of course, such an approach requires to first estimate some bounds on the macroscopic fields that are global in time and space.

Note that the points of $\mathcal{V}$ are not necessarily uniformly distributed, since the grid could be refined only wherever it is necessary and coarsened elsewhere, as it is proposed in [3] for steady flows (with a simple and automatic way to define such a grid). However, for unsteady problems, the situation is more complex. Indeed, first, the estimations of the correct bounds and step of the grid are not necessarily available for every problems (the velocity or the temperature could reach much larger values that were not expected at some times of the simulation), like in complex shock interactions, for instance. Moreover, even if it is possible, this could lead to a grid which is extremely large and dense, hence leading to a very expensive simulation (see an example in section 4.2). Finally, when there are distributions that are very far from their local Maxwellian, their support can be quite different, and there is no analytical way to determine it. This can require several tries to find a correct global velocity grid, which is also expensive.

It is therefore very attractive to try to use a *local* velocity discretization of the distribution function, which means to use *local discrete velocity grids* (LDV) for each time and position. In other words, at each time t and position x, we would like the corresponding distribution $f(t,x,.)$ to be approximated on its own velocity grid, which might be different from the grids used at other times or other positions. The clear advantage of this idea is that we can define an optimally small grid for each distribution, thus we avoid the problems mentioned above. This approach is developed in the next section.

3 A local discrete velocity grid approach

3.1 The method

Now we assume that at time t_n, the distribution function in each space cell $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ is approximated on a set $\mathcal{V}_i^n$ of K local discrete velocities. For simplicity, we assume here that all the local grids have the same number of points K, and the points are uniformly distributed. The first point is denoted by $v_{min,i}^n$ and the last one by $v_{max,i}^n$. That is to say, we have

$$\mathcal{V}_i^n = \left\{ v_{i,k}^n = v_{min,i}^n + (k-1)\Delta v_i^n, \quad k \text{ from 1 to } K \right\}, \qquad \text{where} \qquad \Delta v_i^n = \frac{v_{max,i}^n - v_{min,i}^n}{K-1}.$$

On this local grid, $f(t_n, x_i, .)$ is approximated by K values that are stored in the vector $f_i^n = (f_{i,k}^n)_{k=1}^K$. Each discrete value $f_{i,k}^n$ is an approximation of $f(t_n, x_i, v_{i,k}^n)$.

The corresponding macroscopic quantities $U(t_n, x_i)$ are approximated by U_i^n with the following quadrature formula

$$U_i^n = \langle m f_i^n \rangle_{\mathcal{V}_i^n} = \sum_{k=1}^{K} m(v_{i,k}^n) f_{i,k}^n \omega_k, \tag{7}$$

where the ω_k are the weights of the quadrature. In this paper, the trapezoidal quadrature formula is used: $\omega_1 = \omega_K = 1/2$ and $\omega_k = 1$ for k from 2 to $K-1$.

When one wants to compute an approximation of f at the next time step t_{n+1}, two problems occur. First, how to determine the local discrete velocity grid $\mathcal{V}_i^{n+1}$? We will show below that this can be simply made by using the conservation laws. Second, how to exchange information between two space cells, since the local grids are not the same? This is where we use some interpolation procedure in the method. Let us now describe our algorithm step by step.

Step 1: Macroscopic quantities at t_{n+1}.

We approximate the conservation relation (3) with the following first order upwind scheme

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} \left(\Phi_{i+\frac{1}{2}}^n - \Phi_{i-\frac{1}{2}}^n \right), \tag{8}$$

where the numerical fluxes are defined by

$$\Phi_{i+\frac{1}{2}}^n = \left\langle v^+ m f_i^n \right\rangle_{\mathcal{V}_i^n} + \left\langle v^- m f_{i+1}^n \right\rangle_{\mathcal{V}_{i+1}^n}, \tag{9}$$

which is indeed an approximation of the flux $\left\langle v m f(t_n, x_{i+\frac{1}{2}}) \right\rangle$ at the cell interface. Here, we use the standard notation $v^\pm = (v \pm |v|)/2$. Note that each half flux is computed on the local velocity grid of the corresponding distribution. The vector U_i^{n+1} is an approximation of $U(t_{n+1}, x_i)$, and we note u_i^{n+1} and T_i^{n+1} the corresponding velocity and temperature.

Step 2: discrete velocity grid $\mathcal{V}_i^{n+1}$.

We define this grid by using the new velocity and temperature u_i^{n+1} and T_i^{n+1} to get the bounds

$$v_{min,i}^{n+1} = u_i^{n+1} - 4\sqrt{RT_i^{n+1}} \quad \text{and} \quad v_{max,i}^{n+1} = u_i^{n+1} + 4\sqrt{RT_i^{n+1}}. \tag{10}$$

Then the new grid $\mathcal{V}_i^{n+1}$ is defined as in the previous time step, that is to say by

$$\begin{aligned} \mathcal{V}_i^{n+1} = \{v_{i,k}^{n+1} = v_{min,i}^{n+1} + (k-1)\Delta v_i^{n+1}, \quad k \text{ from 1 to } K\}, \\ \text{with } \Delta v_i^{n+1} = (v_{max,i}^{n+1} - v_{min,i}^{n+1})/(K-1). \end{aligned} \tag{11}$$

Step 3: distribution function at time t_{n+1}.

Here, equation (1) is approximated by a first order upwind scheme, with an implicit relaxation term. If the velocity variable is not discretized, we get for every v:

$$\begin{aligned} f_i^{n+1}(v) = f_i^n(v) - \frac{\Delta t}{\Delta x} v^+ (f_i^n(v) - f_{i-1}^n(v)) - \frac{\Delta t}{\Delta x} v^- (f_{i+1}^n(v) - f_i^n(v)) \\ + \frac{\Delta t}{\tau_i^{n+1}} (M(U_i^{n+1})(v) - f_i^{n+1}(v)). \end{aligned}$$

If now we take into account that each distribution f_i^{n+1}, f_i^n, f_{i-1}^n, and f_{i+1}^n are defined on their own local velocity grid, this scheme must be modified by using a reconstruction procedure.

The discrete distributions f_i^n, f_{i-1}^n, and f_{i+1}^n are used to reconstruct piecewise continuous in velocity functions $\bar{f}_i^n$, $\bar{f}_{i-1}^n$, and $\bar{f}_{i+1}^n$ that are defined as follows:

$$\bar{f}_i^n(v) = \begin{cases} p_i^n(v) & \text{if } v_{min,i}^n \le v \le v_{max,i}^n \\ 0 & \text{else,} \end{cases} \tag{12}$$

where p_i^n is a piecewise continuous function of v constructed through the values $(v_{i,k}^n, f_{i,k}^n)_{k=1}^K$, like a piecewise interpolated polynomial. Since any kind of interpolation could be used, this reconstruction will be discussed in section 3.3. Then we define the discrete values of f_i^{n+1} on its grid $\mathcal{V}_i^{n+1}$ by

$$\begin{aligned} f_{i,k}^{n+1} = \bar{f}_i^n(v_{i,k}^{n+1}) - \frac{\Delta t}{\Delta x} v_{i,k}^{n+1+} (\bar{f}_i^n(v_{i,k}^{n+1}) - \bar{f}_{i-1}^n(v_{i,k}^{n+1})) - \frac{\Delta t}{\Delta x} v_{i,k}^{n+1-} (\bar{f}_{i+1}^n(v_{i,k}^{n+1}) - \bar{f}_i^n(v_{i,k}^{n+1})) \\ + \frac{\Delta t}{\tau_i^{n+1}} (M_k(U_i^{n+1}) - f_{i,k}^{n+1}), \end{aligned} \tag{13}$$

for $k = 1$ to K.

Our scheme is then given by relations (8–13). Now, we give some properties of this scheme.

Property 3.1. *For scheme (8–13), the global mass, momentum, and energy are constant (the scheme is conservative):*

$$\sum_i U_i^n \Delta x = \sum_i U_i^0 \Delta x.$$

Proof. This is a direct consequence of the discretization of the conservation laws (8) with a conservative scheme: indeed, when we take the sum of (8) for every i, the sum of the numerical fluxes cancels out, and we obtain that the total quantities do not change during one time step. This gives the result. □

Even if this property is obvious, we believe it deserves to be noted: first, we point out that the scheme is not given by (8) only, but by all the relations between (8) and (13). Then relation (8) has to be seen as macroscopic conservation laws in which the fluxes are computed by using the discrete kinetic equation (13). Even if (13) is not conservative, the use of (8) implies that the macroscopic mass, momentum, and energy densities are conserved. This is a property shared by several recent schemes based on a dual macro-micro time evolutions or IMEX methods, see for instance [21, 4, 11].

Property 3.2. *Assume that for every cell i, f_i^n is non negative at each point of its local velocity grid and that the corresponding reconstructed piecewise function $\bar{f}_i^n$ is non negative for every v. Then, under the CFL condition $\Delta t \leq \Delta x / \max_{i,k}(|v_{i,k}^{n+1}|)$, $f_{i,k}^{n+1}$ is non negative at each point of its local velocity grid, for every space cell.*

Proof. As it is standard for the upwind scheme for convection problems, it is sufficient to note that (13) can be written as a linear combination of $\bar{f}_i^n$, $\bar{f}_{i-1}^n$, $\bar{f}_{i+1}^n$, and $M(U_i^{n+1})$. The CFL condition of the proposition ensures that the coefficients of this combination are non negative, which gives the result. □

We point out that, while the result of this property is rather standard, it is in fact quite weak here. Indeed, first, the non negativeness of the distribution is obtained only if the reconstruction step preserves the non negativeness of the f_i^n. This is true for linear interpolation, but it is not for many higher order reconstructions. Moreover, this property itself is not sufficient to ensure that the sequence f_i^n can be defined at every time step: indeed, step 2 requires T_i^{n+1} to be non-negative to define the local grid $\mathcal{V}_i^{n+1}$. Unfortunately, it seems hardly possible to prove that this property is true for the scheme presented above. This why a modified schemes are presented in the next section.

Finally, we want to comment on the choice of the time step in this scheme. Indeed, note that, according to property 3.2, step 3 requires a time step defined through the local grids $\mathcal{V}_i^{n+1}$ at time t_{n+1} to correctly define f_i^{n+1}. However, this time step is already needed at step 1 to define U_i^{n+1}, while at this step, $\mathcal{V}_i^{n+1}$ is not already known. This means that we have to use a single time step for steps 1 and 3 that also satisfies the CFL condition based on $\mathcal{V}_i^{n+1}$. A simple algorithm is the following:

(a) We choose $\Delta t_1 = \Delta x / \max_{i,k}(|v_{i,k}^n|)$

(b) We do step 1 and step 2.

(c) For step 3, we compute $\Delta t_2 = \Delta x / \max_{i,k}(|v_{i,k}^{n+1}|)$:

- if $\Delta t_2 > \Delta t_1$, then f^{n+1} can be advanced with Δt_1

- if $\Delta t_2 < \Delta t_1$, then we set $\Delta t_1 = \Delta t_2$, we do not compute f^{n+1} but we directly go back to (b) (steps 1 and 2 of the scheme are done again)

However, note that in practice, we do not need this algorithm: we always use $\Delta t_1 = \Delta x / \max_{i,k}(|v_{i,k}^n|)$ without any stability problem. Indeed, we carefuly checked the sign of the solution at each time step and at every space and velocity point, for all the test cases presented in this paper: we did not observe any loss of positivity and any stability problem.

3.2 Modified versions of the scheme

First, note that if we compute the moments of f_i^{n+1} after step 3, we do not recover the moments U_i^{n+1} defined at step 1. Indeed, according to (13) we have

$$\begin{aligned}
\left\langle m f_i^{n+1} \right\rangle_{\mathcal{V}_i^{n+1}} &= \sum_{\mathcal{V}_i^{n+1}} m(v_{i,k}^{n+1}) f_{i,k}^{n+1} \omega_k \\
&= \sum_{\mathcal{V}_i^{n+1}} m(v_{i,k}^{n+1}) \bar{f}_i^n(v_{i,k}^{n+1}) \omega_k - \frac{\Delta t}{\Delta x} \left(\sum_{\mathcal{V}_i^{n+1}} m(v_{i,k}^{n+1}) (v_{i,k}^{n+1^+} \bar{f}_i^n(v_{i,k}^{n+1}) + v_{i,k}^{n+1^-} \bar{f}_{i+1}^n(v_{i,k}^{n+1})) \omega_k \right. \\
&\qquad \left. - \sum_{\mathcal{V}_i^{n+1}} m(v_{i,k}^{n+1}) (v_{i,k}^{n+1^+} \bar{f}_{i-1}^n(v_{i,k}^{n+1}) - v_{i,k}^{n+1^-} \bar{f}_i^n(v_{i,k}^{n+1})) \omega_k \right) \\
&\quad + \frac{\Delta t}{\tau_i^{n+1}} \left(U_i^{n+1} - \left\langle m f_{i,k}^{n+1} \right\rangle_{\mathcal{V}_i^{n+1}} \right).
\end{aligned}$$

If we compare the terms of this expression to the definition of U_i^{n+1} given by (8) and (9), we find the two vectors cannot be equal. The reason is that in the first expression, we have several quantities on the form $\sum_{\mathcal{V}_i^{n+1}} \phi(v_{i,k}^{n+1}) \bar{f}_i^n(v_{i,k}^{n+1}) \omega_k$, while in the second expression, these quantities are $\sum_{\mathcal{V}_i^n} \phi(v_{i,k}^n) f_{i,k}^n \omega_k$, and they are not equal in general since the grids $\mathcal{V}_i^{n+1}$ and $\mathcal{V}_i^n$ are different. Of course, these quantities are close, since they approximate the same values, but they are not equal.

This means that we have two different approximations of the same macroscopic values: U_i^{n+1} and the moments of f_i^{n+1}. We have numerically compared these quantities and there is indeed no significant difference. However, this difference suggests a modification of the scheme: after step 3, we add one more step in which we define $U_i^{n+1,\star} = \left\langle m f_i^{n+1} \right\rangle_{\mathcal{V}_i^{n+1}}$, and U_i^n is replaced by $U_i^{n,\star}$ in step 1. Then the modified scheme (called the "moment correction method") is the following:

<u>*Step 1:*</u> Macroscopic quantities at t_{n+1}.

$$U_i^{n+1} = U_i^{n,\star} - \frac{\Delta t}{\Delta x} \left(\Phi_{i+\frac{1}{2}}^n - \Phi_{i-\frac{1}{2}}^n \right), \tag{14}$$

where the numerical fluxes are defined by

$$\Phi^n_{i+\frac{1}{2}} = \left\langle v^+ m f^n_i \right\rangle_{\mathcal{V}^n_i} + \left\langle v^- m f^n_{i+1} \right\rangle_{\mathcal{V}^n_{i+1}}, \tag{15}$$

<u>*Step 2:*</u> discrete velocity grid $\mathcal{V}^{n+1}_i$ (step unchanged).

$$v^{n+1}_{min,i} = u^{n+1}_i - 4\sqrt{RT^{n+1}_i} \quad \text{and} \quad v^{n+1}_{max,i} = u^{n+1}_i + 4\sqrt{RT^{n+1}_i}. \tag{16}$$

$$\begin{aligned} \mathcal{V}^{n+1}_i = \{ v^{n+1}_{i,k} = v^{n+1}_{min,i} + (k-1)\Delta v^{n+1}_i, \quad k \text{ from 1 to } K\}, \\ \text{with } \Delta v^{n+1}_i = (v^{n+1}_{max,i} - v^{n+1}_{min,i})/(K-1). \end{aligned} \tag{17}$$

<u>*Step 3:*</u> distribution function at time t_{n+1} (step unchanged).

$$\begin{aligned} f^{n+1}_{i,k} = \bar{f}^n_i(v^{n+1}_{i,k}) - \frac{\Delta t}{\Delta x} v^{n+1+}_{i,k} (\bar{f}^n_i(v^{n+1}_{i,k}) - \bar{f}^n_{i-1}(v^{n+1}_{i,k})) - \frac{\Delta t}{\Delta x} v^{n+1-}_{i,k} (\bar{f}^n_{i+1}(v^{n+1}_{i,k}) - \bar{f}^n_i(v^{n+1}_{i,k})) \\ + \frac{\Delta t}{\tau^{n+1}_i}(M_k(U^{n+1}_i) - f^{n+1}_{i,k}), \end{aligned} \tag{18}$$

for $k = 1$ to K.

<u>*Step 4:*</u> Moment correction step.

$$U^{n+1,\star}_i = \left\langle m f^{n+1}_i \right\rangle_{\mathcal{V}^{n+1}_i} = \sum_{k=1}^{K} m(v^{n+1}_{i,k}) f^{n+1}_{i,k} \omega_k. \tag{19}$$

This means that the macroscopic quantities at time t_{n+1} are modified to be the moments of f^{n+1}_i, and that the discrete conservation laws at the next time step are initialized with these moments. This is similar to a technique used in the "moment guided" method proposed in [10].

For this modified scheme, the non-negativeness property 3.2 is still true, but unfortunately, the conservation property 3.1 is lost: Indeed, even if we deduce from the discrete conservation laws (14) that

$$\sum_i U^{n+1}_i \Delta x = \sum_i U^{n,\star}_i \Delta x,$$

there is no way to link the corrected moment $U^{n,\star}_i$ to the moment vector U^n_i obtained at the previous time step, for the same reason as given at the beginning of this section. Indeed, it is likely that $U^{n,\star}_i$ is different from U^n_i, even if they approximate the same value. Consequently, the scheme is not conservative anymore.

Finally, we conclude this section by another modification that ensures the positivity of the temperature T^{n+1}_i in the previous modified scheme. We propose to replace the quadratures used to compute the macroscopic vector $U^{n,\star}_i$ and the numerical flux $\Phi^n_{i+\frac{1}{2}}$ (see (19) and (15)) by the exact integral of the corresponding reconstructed functions, that is to say:

- in step 1, (15) is replaced by

$$\Phi^n_{i+\frac{1}{2}} = \left\langle v^+ m \bar{f}^n_i \right\rangle + \left\langle v^- m \bar{f}^n_{i+1} \right\rangle ,$$

- in step 4, (19) is replaced by

$$U^{n,\star}_i = \left\langle m \bar{f}^n_i \right\rangle ,$$

where we remind that $\langle \phi \rangle = \int_{\mathbb{R}} \phi(v)\, dv$ for any velocity dependent function. If the reconstruction procedure uses a polynomial interpolation, these integrals are just integrals of piecewise polynomial functions and can be evaluated explicitly. With this definition, the discrete conservation law (14) reads

$$U^{n+1}_i = \left\langle m \Big((1 - \frac{\Delta t}{\Delta x}|v|) \bar{f}^n_i + \frac{\Delta t}{\Delta x} v^+ \bar{f}^n_{i-1} - \frac{\Delta t}{\Delta x} v^- \bar{f}^n_{i+1} \Big) \right\rangle = \langle m\phi \rangle$$

where ϕ is a piecewise continuous function of v. Now we have the following property.

Property 3.3. *Under the CFL condition $\Delta t \leq \Delta x / \max_{i,k}(|v^n_{i,k}|)$, the function ϕ is non negative, and hence T^{n+1}_i is positive.*

Proof. Observe that ϕ is a linear combination of $\bar{f}^n_i$, $\bar{f}^n_{i-1}$, $\bar{f}^n_{i+1}$. The last two coefficients are always non negative. As a consequence of the CFL condition, the first coefficient, which is $1 - \frac{\Delta t}{\Delta x}|v|$, is non negative if $|v|$ is small enough (that is to say $|v| \leq \max_{i,k}(|v^n_{i,k}|)$). If v is larger, the coefficient is negative, but by construction $\bar{f}^n_i(v) = 0$ (see (12)). Consequently, ϕ is non negative for every v, and hence U^{n+1}_i is realized by a non negative distribution. It is then a standard result that the corresponding density, energy and temperature are positive. □

However, we observe that in practice, the first modified scheme (14–19) preserves the positivity. This is why we do not use this second modified scheme in the numerical tests presented in this paper.

3.3 Reconstruction: from $f^n_{i,k}$ to $\bar{f}^n_i$

To compute $\bar{f}^n_i(v^{n+1}_{i,k})$ in equation (13), we have to use a reconstruction procedure. First, if $v^{n+1}_{i,k}$ is external to $\mathcal{V}^n_i$, we set $\bar{f}^n_i(v^{n+1}_{i,k}) = 0$: indeed, if the grid $\mathcal{V}^n_i$ is large enough, the distribution is very very small outside the grid, and it is reasonable to set it to 0. If $v^{n+1}_{i,k}$ is inside $\mathcal{V}^n_i$, it is not a node of $\mathcal{V}^n_i$ in general, and we use a piecewise polynomial interpolation. We observed that first order polynomial interpolation is not accurate enough (a lot of discrete velocities are needed to get correct results). However, higher order interpolation produces oscillations, especially in very rarefied regimes, which is probably due to the large velocity gradients (and even discontinuities) of the distribution functions in such regimes.

Consequently, we use the essentially non oscillatory (ENO) interpolation (see [24] or [13]): with 3 or 4 point interpolation, the accuracy is good and there is almost no oscillation.

The reconstruction algorithm is summarized below.

1. If $|v_{i,k}^{n+1}| > \max(|v_{min,i}^n|, |v_{max,i}^n|)$, then set $\bar{f}_i^n(v_{i,k}^{n+1}) = 0$
2. else
   (a) find the interval $[v_{i,k'}^n, v_{i,k'+1}^n]$ inside $\mathcal{V}_i^n$ that contains $v_{i,k}^{n+1}$
   (b) compute the q point ENO polynomial function P defined on the stencil $\{v_{i,k'-(q-1)}^n, v_{i,k'+q}^n\}$
   (c) set $\bar{f}_i^n(v_{i,k}^{n+1}) = P(v_{i,k}^{n+1})$

Of course, the same procedure is applied to the other reconstructed values $\bar{f}_{i+1}^n(v_{i,k}^{n+1})$ and $\bar{f}_{i-1}^n(v_{i,k}^{n+1})$ in (13).

Remark 3.1. If we use a first order interpolation (linear reconstruction), the positivity of the distribution function is preserved, this can be proved easily. But, for the higher order ENO interpolation that we use in practice, there is no reason why the positivity should always be preserved. It could be interesting to look for modified interpolations that preserve positivity. However in all the test cases that have been studied here, this drawback does not induces a loss of positivity of f_i^{n+1} in (13).

3.4 Non symmetric local discrete velocity grids

When the flow is far from equilibrium, the distribution functions are different from their local Maxwellian, and might have a non symmetric shape. In particular, their support might be non symmetric as well (see for instance the heat transfer problem in the rarefied regime as shown in section 4.3). However, the local grids defined in section 3.1 are based on the local Maxwellians and are necessarily symmetric. In this section, we propose a method to modify the grid if necessary. This method can be applied to both versions (8–13) and (14–19) of our scheme.

First, note that up to now, we have defined uniform local grids with a constant number of points. However, the method is readily extended to non uniform grids with a variable number of points : we just have to replace K by K_i^n ad ω_k by $\omega_{i,k}^n$ in every expressions of section 3.1.

Then, the idea is to enlarge the grid $\mathcal{V}_i^{n+1}$ if $f_{i,k}^{n+1}$ is not small enough at its boundaries. This is made by using a splitting between the relaxation step and the transport step: we first compute the intermediate quantity $f_{i,k}^{n+1/2}$ by using the transport equation as

$$f_{i,k}^{n+1/2} = \bar{f}_i^n(v_{i,k}^{n+1}) - \frac{\Delta t}{\Delta x} v_{i,k}^{n+1+}(\bar{f}_i^n(v_{i,k}^{n+1}) - \bar{f}_{i-1}^n(v_{i,k}^{n+1})) - \frac{\Delta t}{\Delta x} v_{i,k}^{n+1-}(\bar{f}_{i+1}^n(v_{i,k}^{n+1}) - \bar{f}_i^n(v_{i,k}^{n+1})), \tag{20}$$

for $k = 1$ to K. At the end of the transport step, the values of the distribution function $f_i^{n+1/2}$ at the boundary points $v_{i,max}^{n+1}$ and $v_{i,min}^{n+1}$ of $\mathcal{V}_i^{n+1}$ are compared to the maximum value of the distribution in the grid: if the relative difference between one of these boundary values and the maximum value in the grid is larger than a tolerance (that was taken to 10^{-4} in our tests), then new grid points $w_R = v_{i,max}^{n+1} + \Delta v_i^{n+1}$ or $w_L = v_{i,min}^{n+1} - \Delta v_i^{n+1}$ are added outside

the grid, and the corresponding values of $f_{i,k}^{n+1/2}$ are computed by using (20) again. This step is repeated until the left and right relative differences are smaller than the specified tolerance. At the end of this step, the modified grid $\mathcal{V}_i^{n+1}$ now has K_i^{n+1} velocities. Finally, $f_{i,k}^{n+1}$ is obtained from the relaxation step through the relation

$$f_{i,k}^{n+1} = f_{i,k}^{n+1/2} + \frac{\Delta t}{\tau_i^{n+1}}(M_k(U_i^{n+1}) - f_{i,k}^{n+1}), \tag{21}$$

for $k = 1$ to K_i^{n+1}.

Note that that the method suggested here is just a modification ot the previous schemes. For scheme (8–13), the discrete kinetic equation (13) is replaced by the transport/relaxation splitting (20–21). After the use of the transport step (20) on $\mathcal{V}_i^{n+1}$, it is used iteratively to add new points outside the grid, until the distribution is small enough, which leads to an "enlarged" grid, still denoted by $\mathcal{V}_i^{n+1}$. Then, the relaxation step (21) is used. Scheme (14–19) can be modified accordingly.

It would also be interesting to use an automatic refinement of the local grid around the possible discontinuities, but this is not studied in this paper.

3.5 Extensions to other collision models

This algorithm can be adapted to any collision model which is local in space, like the ES-BGK or Shakhov models, or even the Boltzmann collision operator itself. Indeed, as long as the grids are defined by using the velocity and the temperature, we only have to use the conservation laws (density, momentum, and energy), that are satisfied by all the standard models. The fact that a model like ES-BGK contains non-conservative quantities has no influence on the algorithm.

This is slightly different if one wants to use higher order moments to define the local velocity grids. Indeed, we could imagine that the shear stress and the heat flux, for instance, could also be used to define non isotropic and non symmetric local velocity grids, even if this is not what we advocate now. In that case, we would have to use moment equations that are not conservation laws (evolution of the pressure tensor and the energy flux). Then, the applicability of our algorithm depends on the time approximation of the collision operator. If we use an explicit time discretization, the right-hand side of the higher-order moments equations can be explicitly computed with the distributions at time t_n. However, if we use a semi-implicit time discretization (as we do in this paper), the discrete moment equations can be solved only if the right-hand side can be written as a function of the moment vector at time t_{n+1}: this is true for relaxation models like BGK er ES-BGK and Shakhov models, but this is not true in general (for the Boltzmann collision operator for instance).

However, note that this discussion makes sense only when the velocity is at least of dimension 2 (since ES-BGK model and Boltzmann collision operator do not exist for a one dimensional velocity), which will be studied in a forthcoming work.

4 Numerical results

In this section we present three numerical tests to illustrate the main features of our method (denoted by LDV, for local discrete velocity grid). It is compared to a standard discrete velocity method (with a global velocity grid) denoted by DVM (see [18]). First, the numerical scheme is tested on the Sod test case for three different regimes: the rarefied, fluid, and free transport regimes. The second test is the two interacting blast waves problem in which very high temperature differences make the standard DVM inefficient. The third test case is devoted to the heat transfer problem, where the use of non symmetric local grids is shown to be necessary when the Knudsen number increases. In these tests, the gas constant R is 208.1, except for the free transport regime in section 4.1.3 where $R = 1$.

4.1 Sod test case

4.1.1 Rarefied regime

We consider a classical Sod test in a rarefied regime for the BGK model (1) with the parameters $\omega = -0.19$ and $C = 1.08 \cdot 10^{-9}$ used in the relaxation time τ. The space domain is the interval $[0, 0.6]$ discretized with 300 points. The initial state is given by a local Maxwellian distribution whose macroscopic quantities are

$$\begin{aligned} &T(x) = 0.00480208,\ \rho(x) = 0.0001,\ u(x) = 0 \text{ for } x \in [0, 0.3] \\ &T(x) = 0.00384167,\ \rho(x) = 0.0000125,\ u(x) = 0 \text{ for } x \in]0.3, 0.6]. \end{aligned} \tag{22}$$

The DVM and LDV methods are compared to a reference solution given by the DVM method computed for a large and fine velocity grid (obtained after a convergence study). This velocity grid has 600 points uniformly distributed in the interval $[v_{min}, v_{max}]$ where

$$v_{min} = \min_{t,x}\big(u(t,x) - 6\sqrt{RT(t,x)}\big), \quad v_{max} = \max_{t,x}\big(u(t,x) + 6\sqrt{RT(t,x)}\big), \tag{23}$$

which leads to bounds equal to ± 6. Of course, such bounds cannot be determined a priori, and several computations with larger and larger velocity grids have to be done before the correct bounds are found. This illustrates the difficulty to use a standard DVM when the extreme values of the velocity and the temperature are not known a priori. Indeed, here, the temperature in the shock after the initial time is higher than the two initial left and right temperatures. If the velocity grid is computed with formula (5) and (6) and the bounds are estimated with the initial values of T and u (which gives bounds equal to ± 4) , then the grid is not large enough: the results are not correct, even if the number of velocities is increased so as to reach the grid convergence, which is obtained here with 100 velocities. This is shown in figure 2.

At the contrary, our LDV method dynamically adapts to the time variations of u and T and gives very accurate results with 30 discrete velocities only in each local grid, as it is shown in figure 2. Consequently, the LDV method is very efficient for this case.

Note that in this test, the reconstruction procedure used the 4-points ENO interpolation. See section 4.1.3 for an analysis of the influence of the order of interpolation.

4.1.2 Fluid regime

Now, we consider the same Sod test case, but in the fluid regime. This regime corresponds to the limit case of equation (1) when τ is set to 0. Note that since both DVM and LDV methods are used with a time semi-implicit scheme, taking $\tau = 0$ means that f^{n+1} is set to $M(U^{n+1})$ at each time step (and hence the choice of the interpolation procedure has no influence), and we get two different numerical schemes for the compressible Euler equations of gas dynamics.

Here, the reference DVM has 100 velocities only and bounds equal to ± 5.2 . The DVM with the grid computed with the initial values of T and u has also 100 velocities with bounds equal to ± 4 , but it still gives incorrect values (see figure 3), for the same reasons as mentioned in the previous section. At the contrary, our LDV method gives very accurate results with 10 velocities only.

Note that the results obtained in this fluid regime are very close to those obtained in the rarefied regime (even if the shock profile is stiffer in the fluid regime, as expected). This can be understood by computing the Knudsen number of the rarefied regime. In this test, the initial mean free path is between $3\,10^{-5}$ (left state) and $2\,10^{-4}$ (right state). It is difficult to define a Knudsen number here, since there is no macroscopic length scale, but if we choose the length of the computational domain, we find a Knudsen number between $5\,10^{-5}$ and $3\,10^{-4}$, which is quite small.

4.1.3 Free transport regime

We consider the free transport regime corresponding to the limit case in (1) when τ tends to $+\infty$. In this section, we take $R = 1$ and the standard dimensionless values for the Sod test case. The space domain is $[-1, 1]$ and is discretized with 300 points. The distribution function is initialized by the local Maxwellian distribution function with

$$\begin{aligned} \rho = 1,\ u = 0,\ p = 1 \quad \text{in } [-1, 0[, \\ \rho = 0.125,\ u = 0,\ p = 0.1 \quad \text{in } [0, 1]. \end{aligned} \tag{24}$$

For this test case the numerical results are compared to the analytical solution of the free transport equation.

It is very difficult to accurately approximate the free transport equation with a standard DVM: the macroscopic profiles obtained with the DVM show several plateaux. These plateaux are not due to the space and time approximation, but are only due to the velocity discretization. Indeed, it can be easily proved that the macroscopic profiles of the DVM solution at time t have plateaux of length $t\Delta v$, where Δv is the step of the global uniform grid. This is clearly seen in figures 4–6 (top), where the DVM has 30 discrete velocities with bounds equal to ± 4 . This phenomenon is known as the ray effect that appears with the discrete ordinate approximations of the radiative transfer equation.

When we test this problem with our LDV method, with 2 point piecewise linear interpolation, and 30 velocities in each local grids, the results are very bad: we observe very large oscillations (see figures 4–6, bottom). This is probably due to the fact that this interpolation

is not accurate enough. Then we use 3 and 4 point ENO interpolations, and we observe in the same figures that the solution is now much closer to the exact solution. Moreover, while we have the same number of discrete velocities in each local grid as in the DVM, we observe that the plateaux are completely eliminated.

However, there are still some oscillations in the results obtained with the LDV (note that these oscillations are not amplified and that the numerical solution remains bounded for larger times). The oscillations are probably due to the fact that these results were obtained without the moment correction method. Indeed, if we do now the same simulation with this moment correction method (scheme (14–19)), the results are very good: there are much less oscillations, almost no plateau phenomenon, and the results are much closer to the analytical solution, see figures 7–9.

Up to now, we do not know the reason for these oscillations and it is not clear why they are eliminated when we use the moment correction method. Our intuition is that in the original method, there is some incompatibility between the discretization of the conservation laws and the discretization of the kinetic equation: namely, the moments of the discrete kinetic equation do not lead to the discrete conservation laws that are solved. This is why the discrete conservation laws and the discrete kinetic equation lead to two different approximations of the moment vector at time t_{n+1}. The moment correction method forces these quantities to be equal.

4.2 Two interacting blast waves

This section is devoted to the test case called "the two interacting blast waves" (see [22]). Here, the relaxation time is defined with $\omega = -0.19$ and $C = 1.08\,10^{-9}$. The space domain is the interval $[0, 1]$ which is still discretized with 300 points. The initial distribution function is a local Maxwellian distribution whose macroscopic quantities are given by $\rho = 1$ and $u = 0$ everywhere, and

$$T = 4.8, \text{ in } [0, 0.1], \quad T = 4.8\,10^{-5} \text{ in }]0.1, 0.9], \quad T = 4.8\,10^{-1} \text{ in }]0.9, 1].$$

On the left and right boundaries, we use Neumann boundary conditions: we set the values of f, u, and T in boundary ghost-cells to their values in the corresponding real boundary cells.

Here, the bounds of the global grid of the DVM are determined by the largest initial temperature (we get ± 126.5), and its step size is given by the smallest initial temperature. Then we find that the coarsest global grid that satisfies conditions (5)-(6) has not less than 2 551 velocities! In figures 10–12, we observe that the LDV method requires only 30 velocities to give results that are very close to the DVM method (with 2 551 velocities), both before and after the shock. This proves the high efficiency of the LDV approach for this case. Note that here again, we use a 4 point ENO interpolation in the LDV method.

Finally, we plot in figure 13 some local velocity grids for different space positions: in these plots, each vertical line is a local velocity grid, and its nodes are the small dots on the line. Note that before the waves interaction (top), the velocity grids in the middle of the

domain are much smaller than the grid in the left state, which is due to the different order of magnitude of the temperature at this time. After the interaction, the temperature is more homogeneous, and the grids as well (see the bottom plot in this figure).

4.3 Heat transfer problem

In this test, we consider the evolution of a gas enclosed between two walls kept at temperature $T_L = 300$ and $T_R = 1000$. At these walls, the distribution function satisfies the diffuse boundary condition

$$f(x=0, v>0) = M_{\rho_L,0,T_L}, \quad f(x=1, v<0) = M_{\rho_R,0,T_R} \tag{25}$$

where

$$\rho_L = -\frac{\int_{v<0} v f(x=0,v)dv}{\int_{v>0} v M_{1,0,T_L} dv}, \quad \rho_R = -\frac{\int_{v>0} v f(x=1,v)dv}{\int_{v<0} v M_{1,0,T_R} dv}, \tag{26}$$

and $M_{\rho,0,T}$ denotes $\rho/\sqrt{2\pi RT}\exp(-v^2/2RT)$ for every ρ and T. The initial data is the Maxwellian with density ρ_0 (to be defined later), velocity $u_0 = 0$, and $T_0 = 300$. Here, the relaxation time is defined with $\omega = -0.5$ and $c = 6.15 \cdot 10^{-9}$.

The boundary conditions are taken into account in our numerical scheme by a ghost cell technique, as it is standard in finite volume schemes. Left and right ghost cells are defined for $i = 0$ and $i = i_{max} + 1$, and the velocity grids $\mathcal{V}_0^n$ and $\mathcal{V}_{i_{max}+1}^n$ in these cells are defined so as to correctly describe the corresponding wall Maxwellians. Then, the density ρ_L and ρ_R, that are defined as the ratio of an outgoing mass flux at a wall to the corresponding incoming Maxwellian mass flux, are approximated by using the boundary cell and the corresponding ghost cell, that is to say:

$$\rho_L = -\frac{\langle v^- f_1^n \rangle_{\mathcal{V}_1^n}}{\langle v^+ M(1,0,T_L)\rangle_{\mathcal{V}_0^n}}, \quad \rho_R = -\frac{\langle v^+ f_{i_{max}}^n \rangle_{\mathcal{V}_{i_{max}}^n}}{\langle v^- M(1,0,T_R)\rangle_{\mathcal{V}_{i_{max}+1}^n}}.$$

For this test, we use the moment correction method with fourth order ENO interpolation, except for the computations discussed at the end of this section (see remark 4.1 below). We also use several Knudsen numbers Kn here. This number is parametrized by the initial density ρ_0. We first analyze the LDV method in the transitional regime ($\rho_0 = 1.88862\ 10^{-5}$, which gives $\mathrm{Kn} = 10^{-2}$): here, both the LDV and DVM are converged with 30 velocities (the bounds of the global grid are ± 1825.34), while the space domain $[0, 1]$ is discretized with 1000 points. However, the results obtained with the LDV are not accurate enough (see figure 14). An analysis of this problem shows that this is due to the local grid close to the right boundary which is not large enough: for small times, the distributions at these points are highly non symmetric.

To correct this problem, we use the algorithm proposed in section 3.4 to enlarge the local grids in a non symmetric way. Then, the LDV with 30 velocities now gives results that are indistinguishable from the DVM, see figure 15.

Then, we test the LDV method in the rarefied regime (Kn = 1, $\rho_0 = 1.88862\ 10^{-7}$): the LDV (with enlarged non symmetric local grids) and the DVM are converged with 300 velocities, while the space domain $[0, 1]$ is discretized with 300 points. Here again, both methods give results that are almost indistinguishable (see figure 16). Unfortunately, the number of velocities required to get converged results is very large here, even for the LDV (300 velocities). This is probably due to the fact that the distribution function is discontinuous with respect to the velocity in this test, with very large jumps: our velocity grids, even the local ones, are uniform, and cannot capture these discontinuities when the number of velocities is too small. However, we show in figure 17 the results obtained with 50 velocities only, and we observe that the LDV gives results that are more accurate than the DVM.

Finally, we did the same computations for Kn = 10 ($\rho_0 = 1.88862\ 10^{-8}$) and Kn = 1000 ($\rho_0 = 1.88862\ 10^{-10}$) and we observed the following. First, the plateau phenomenon in the DVM approach with 100 velocities is clearly seen with Kn= 10 (while it was only slightly visible for Kn = 1). For Kn = 1000, the results are almost the same. For the LDV, when the number of discrete velocities is the same as for the DVM, the results are close to the reference solution (no plateau, no oscillations) for Kn = 10 and Kn = 1000, which is much better than with the DVM (see figures 18 and 19). When the number of velocities is not large enough (30 points tested here), both method give wrong results, even if the LDV is better.

Remark 4.1. We also compare our LDV method with and without the moment correction step, for P1 and fourth order ENO interpolation. We do not find it usefull to add the corresponding curves in this paper, but our observations are summarized below:

- for Kn = 0.01, there is not much difference if the moment correction method is used or not:
  - with fourth order ENO interpolation, both methods give good results, even if we note a solution which is slightly less smooth without the moment correction step (there are a few small peaks).
  - if the P1 interpolation is used, both methods give a wrong solution (with small oscillations without the moment correction method).
- for larger Kn, (Kn $= 1, 10, 1000$):
  - if the moment correction method is not used, we observe oscillations whose amplitude increases with Kn, regardless of the interpolation.
  - with the moment correction method and the P1 interpolation, the difference between the numerical results and the reference solution increases with Kn, except if the number of discrete velocities is increased too.

4.4 CPU time comparisons

We have compared the CPU cost of our method (on a single processor Pentium(R) Dual-Core CPU E65002.9GHz) to the standard DVM with a global grid, by using the fortran

subroutine `cpu_time`, and the following test cases:

- Sod test: we compared the DVM with 30 discrete velocities (shown in figures 4–6 (top) to our LDV with 30 points, 4 points ENO interpolation, and the moment correction method (shown in figures 7–9);
- Blast waves: test case shown in figures 10–12 (bottom);
- Heat transfer: comparison between the LDV with 50 velocities and non symmetric grids, to the DVM with 50 velocities (see figure 17).

We observed (see table 1) that our method with local velocity grids is more expensive than the global grid method for Sod et heat transfer tests. Since the number of velocities in the grids is smaller with our method, this increase in CPU cost is probably due to the very large number of interpolations made in the evaluation of reconstructed distributions. At the contrary, for the blast wave problem, the number of velocities is so large in the global grid that our method is less expensive. However, as expected, the gain factor in CPU time (which is 45) is smaller than the gain factor in number of velocities (which is 85).

We point out that the implementation of our method has not been optimized in this work, and such an optimization would probably make the method faster. However, these comparisons show that our algorithms have to be improved to be less computationally expensive, in particular to reduce the cost of the reconstructions of the distribution in their local grids. This is now investigated in a forthcoming work for 2D problems.

5 Conclusion and perspectives

We have presented a new velocity discretization of kinetic equations of rarefied gas dynamics: in this method, the distribution functions are discretized with velocity grids that are local in time and space, contrary to standard discrete velocity or discrete ordinate methods. The local grids dynamically adapt to time and space variations of the support of the distribution function, by using the conservation laws.

This method is very efficient in case of strong variations of the temperature, for which a standard discrete velocity method requires a very large number of velocities. Moreover, it allows to eliminate the plateau phenomenon in very rarefied regimes.

We mention that in this study, the space discretization is a simple first order upwind method, which is known to have a very low accuracy. However, our method is quite independent of the space approximation: any higher order finite volume or finite difference approximation could be used. For instance, a second order upwind scheme with limiters can be used very easily by adding a flux limiter in (8) and slope limiters in (12). However, in this preliminary work, we find it simpler to use a first order scheme to analyze the properties of the method, and to compare its advantages and drawbacks. We defer the investigation of higher order schemes to a work in progress in which our method will be extended to multi-dimensional problems and its computational cost will be reduced.

Moreover, several aspects of the method should be better understood, in particular, why are there some oscillations if the moment correction method is not used, in the rarefied and free transport regimes, even with high order ENO interpolation? A mathematical analysis of the numerical method could be interesting here.

Acknowledgements. This study has been carried out in the frame of "the Investments for the future" Programme IdEx Bordeaux – CPU (ANR-10-IDEX-03-02).

References

[1] V.V. Aristov. Method of adaptative meshes in velocity space for the intense shock wave problem. *USSR J. Comput. Math. Math. Phys.*, 17(4):261–267, 1977.

[2] C. Baranger, J. Claudel, N. Herouard, and L. Mieussens. Locally refined discrete velocity grids for deterministic rarefied flow simulations. *AIP Conference Proceedings*, 1501(1):389–396, 2012.

[3] C. Baranger, J. Claudel, N. Hérouard, and L. Mieussens. Locally refined discrete velocity grids for stationary rarefied flow simulations. *Journal of Computational Physics*, 257, Part A(0):572 – 593, 2014.

[4] Mounir Bennoune, Mohammed Lemou, and Luc Mieussens. Uniformly stable numerical schemes for the boltzmann equation preserving the compressible navier–stokes asymptotics. *Journal of Computational Physics*, 227(8):3781 – 3803, 2008.

[5] G.A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows.* Oxford Science Publications, 1994.

[6] A. V. Bobylev and S. Rjasanow. Fast deterministic method of solving the Boltzmann equation for hard spheres. *Eur. J. Mech. B Fluids*, 18(5):869–887, 1999.

[7] A.V. Bobylev, A. Palczewski, and J. Schneider. A Consistency Result for a Discrete-Velocity Model of the Boltzmann Equation. *Siam J. Numer. Anal.*, 34(5):1865–1883, 1997.

[8] C. Buet. A Discrete-Velocity Scheme for the Boltzmann Operator of Rarefied Gas Dynamics. *Transp. Th. Stat. Phys.*, 25(1):33–60, 1996.

[9] S. Chen, K. Xu, C. Lee, and Q. Cai. A unified gas kinetic scheme with moving mesh and velocity space adaptation. *Journal of Computational Physics*, 231(20):6643 – 6664, 2012.

[10] Pierre Degond, Giacomo Dimarco, and Lorenzo Pareschi. The moment-guided Monte Carlo method. *Internat. J. Numer. Methods Fluids*, 67(2):189–213, 2011.

[11] G. Dimarco and L. Pareschi. Asymptotic preserving implicit-explicit Runge-Kutta methods for nonlinear kinetic equations. *SIAM J. Numer. Anal.*, 51(2):1064–1087, 2013.

[12] F. Filbet and T. Rey. A Rescaling Velocity Method for Dissipative Kinetic Equations - Applications to Granular Media. 27 pages, 2012.

[13] U. Fjordholm, S. Mishra, and E. Tadmor. Eno reconstruction and eno interpolation are stable. *Foundations of Computational Mathematics*, 13:139–159, 2013.

[14] J.R.Haack and I.M. Gamba. Conservative deterministic spectral boltzmann solver near the grazing collisions limit. *AIP Conference Proceedings*, 2012.

[15] V.I. Kolobov and R.R. Arslanbekov. Towards adaptive kinetic-fluid simulations of weakly ionized plasmas. *Journal of Computational Physics*, 231(3):839 – 869, 2012.

[16] V.I. Kolobov, R.R. Arslanbekov, V.V. Aristov, A.A. Frolova, and S.A. Zabelok. Unified solver for rarefied and continuum flows with adaptive mesh and algorithm refinement. *Journal of Computational Physics*, 223(2):589 – 608, 2007.

[17] V.I. Kolobov, R.R. Arslanbekov, and A.A. Frolova. Boltzmann solver with adaptive mesh in velocity space. In *27th International Symposium on Rarefied Gas Dynamics*, volume 133 of *AIP Conf. Proc.*, pages 928–933. AIP, 2011.

[18] L. Mieussens. Discrete Velocity Model and Implicit Scheme for the BGK Equation of Rarefied Gas Dynamics. *Math. Models and Meth. in Appl. Sci.*, 8(10):1121–1149, 2000.

[19] L. Mieussens. Discrete-velocity models and numerical schemes for the Boltzmann-BGK equation in plane and axisymmetric geometries. *J. Comput. Phys.*, 162:429–466, 2000.

[20] V.A. Panferov and A. G. Heintz. A new consistent discrete-velocity model for the boltzmann equation. *Mathematical Methods in the Applied Sciences*, 25(7):571–593, 2002.

[21] Sandra Pieraccini and Gabriella Puppo. Implicit–explicit schemes for bgk kinetic equations. *Journal of Scientific Computing*, 32:1–28, 2007.

[22] P.Woodward and P.Colella. The numerical simulation of two-dimensional fluid flow with strong shocks. *J. Comput. Phys.*, 54:115–173, 1984.

[23] F. Rogier and J. Schneider. A Direct Method For Solving the Boltzmann Equation. *Transp. Th. Stat. Phys.*, 23(1-3):313–338, 1994.

[24] C.-W. Shu. Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws. Technical Report 97-65, ICASE, 1997.

[25] S. Takata, Y. Sone, and K. Aoki. Numerical analysis of a uniform flow of a rarefied gas past a sphere on the basis of the boltzmann equation for hard-sphere molecules. *Physics of Fluids A: Fluid Dynamics*, 5(3):716–737, 1993.

[26] V. A. Titarev. Efficient deterministic modelling of three-dimensional rarefied gas flows. *Communications in Computational Physics*, 12(1):162–192, 2012.

[27] K. Xu and J.-C. Huang. A unified gas-kinetic scheme for continuum and rarefied flows. *J. Comput. Phys.*, 229:7747–7764, 2010.

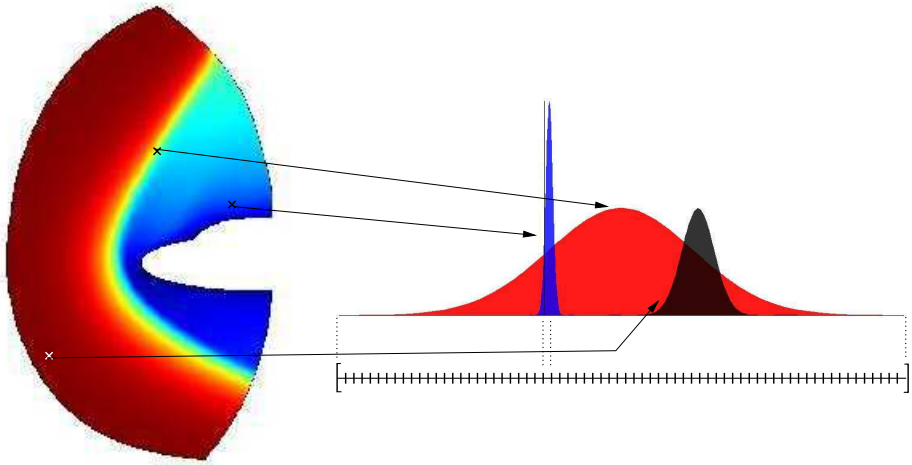

Figure 1: Three distribution functions in different space points of a computational domain for a re-entry problem, and the corresponding global discrete velocity grid $\mathcal{V}$.

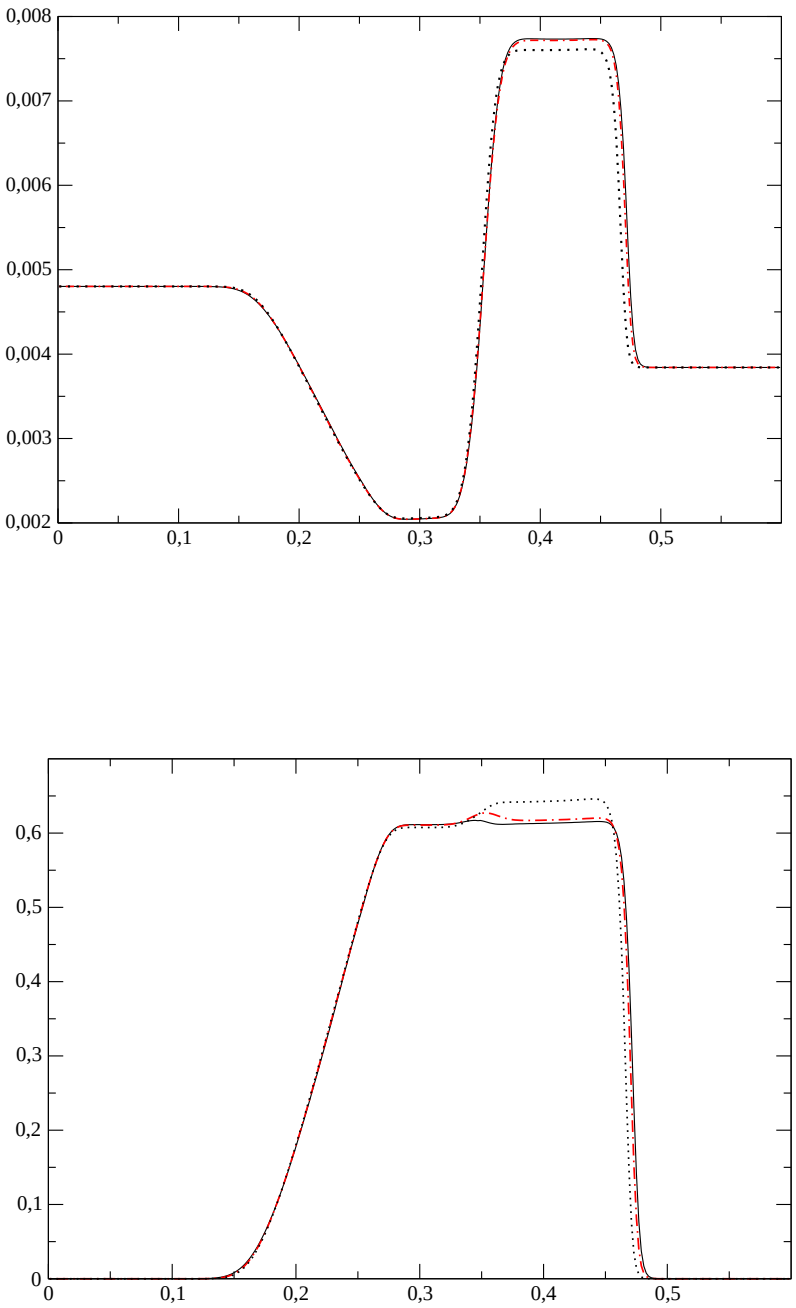

Figure 2: Sod test case, rarefied regime: temperature (top) and velocity (bottom) profiles, at time 7.34 10^{-2}. The solid line is the reference solution obtained with the DVM with the enlarged global grid (600 points), the dotted line is the DVM with an incorrect grid (100 points), while the dot-dashed line is the LDV method (30 points).

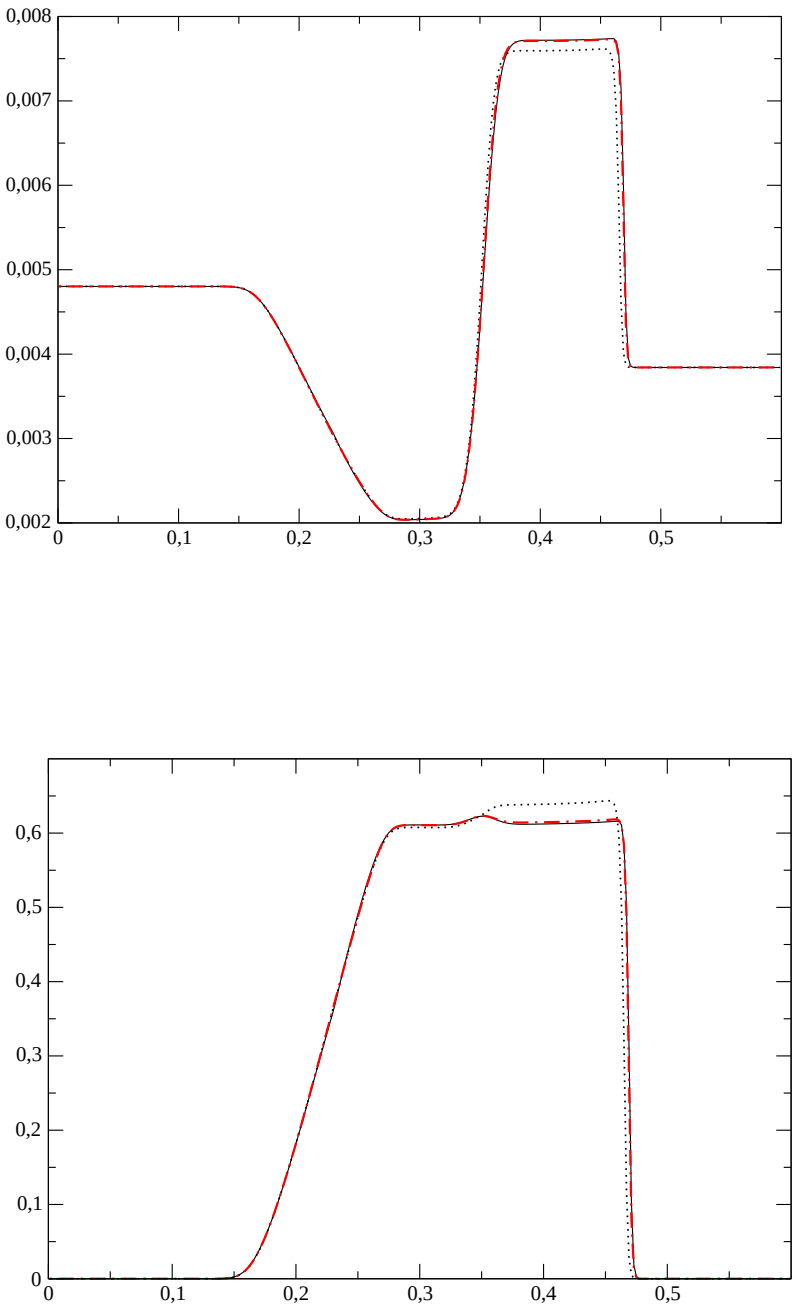

Figure 3: Sod test case, fluid regime: temperature (top) and velocity (bottom) profiles, at time 7.34 10^{-2}. The solid line is the reference solution obtained with the DVM with the enlarged global grid (100 points), the dotted line is the DVM with an incorrect grid (100 points), while the dot-dashed line is the LDV method (10 points).

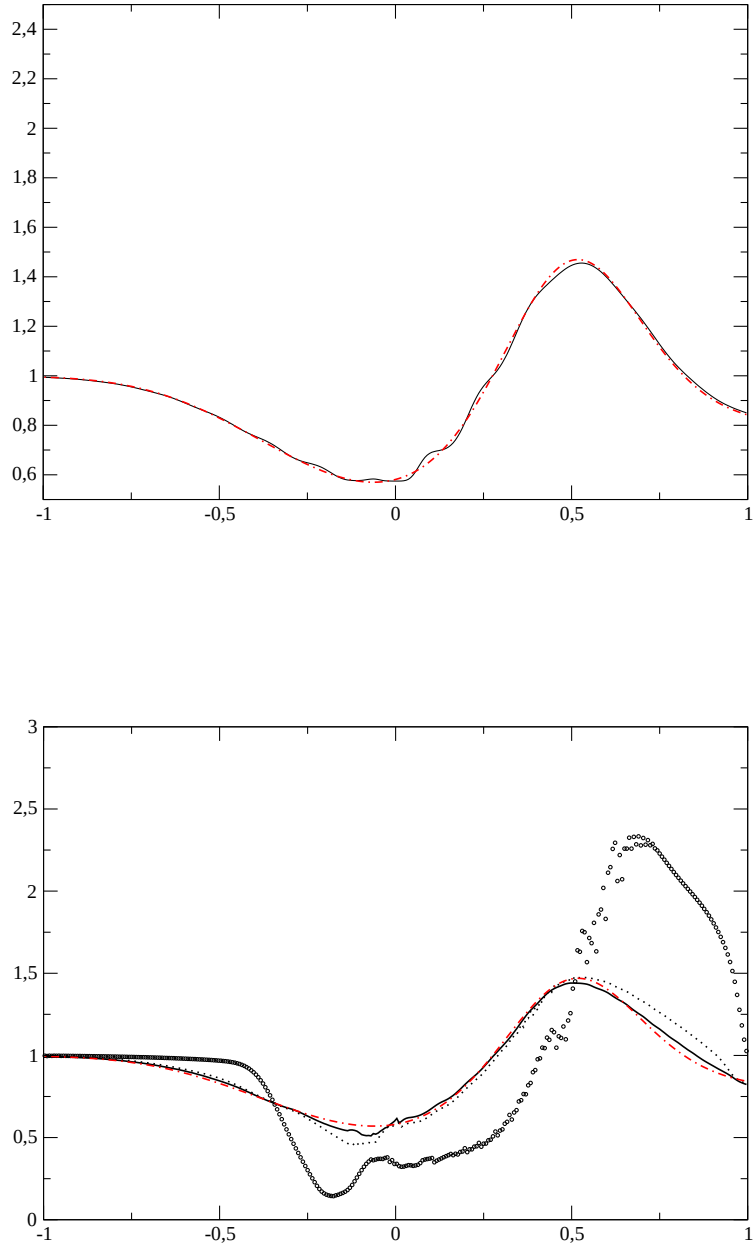

Figure 4: Sod test case, free transport: temperature at time 0.3. Top: comparison between the exact solution (dot-dashed) and with a 30 points DVM (solid). Bottom, comparison between the exact solution (dot-dashed) and several LDVs with 30 points: with first order interpolation ('o'), with 3 points-ENO (dotted), with 4 points-ENO (solid).

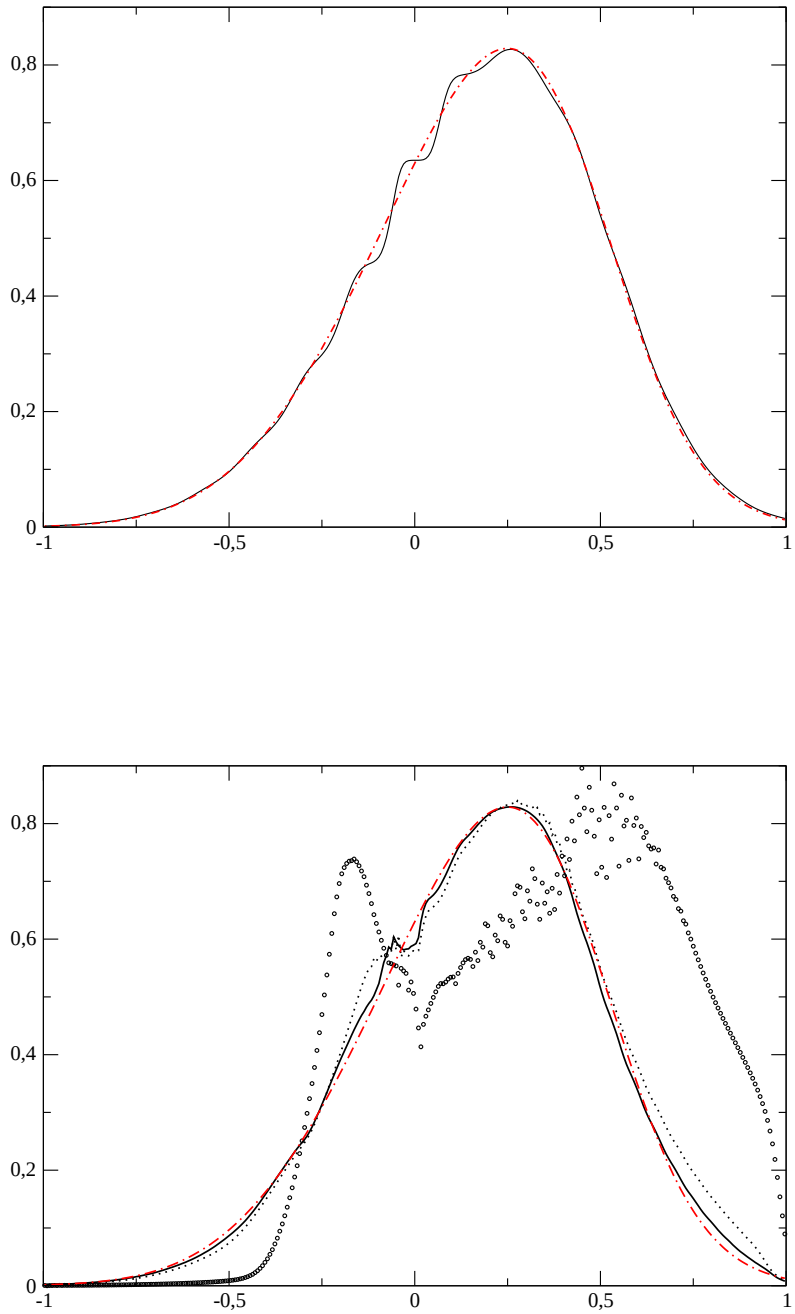

Figure 5: Same as figure 4 for the velocity.

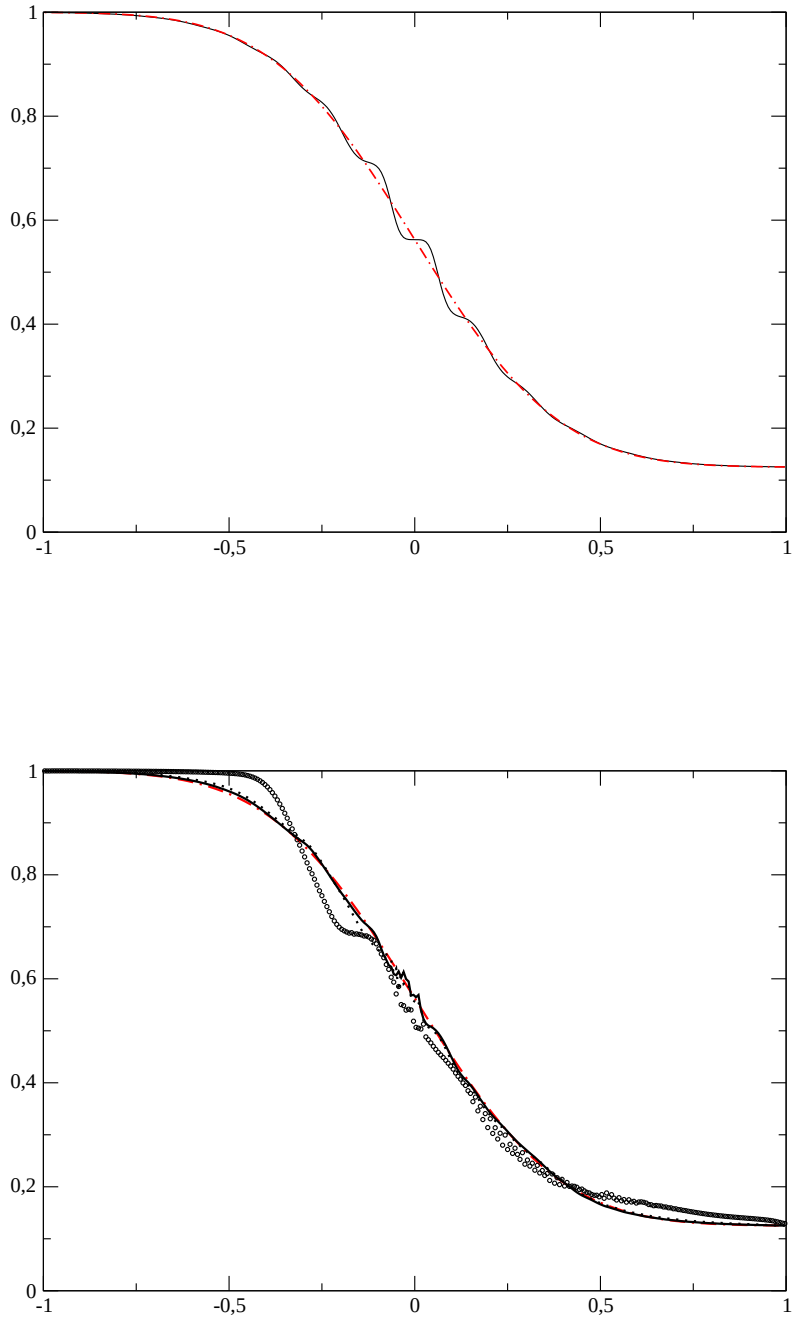

Figure 6: Same as figure 4 for the density.

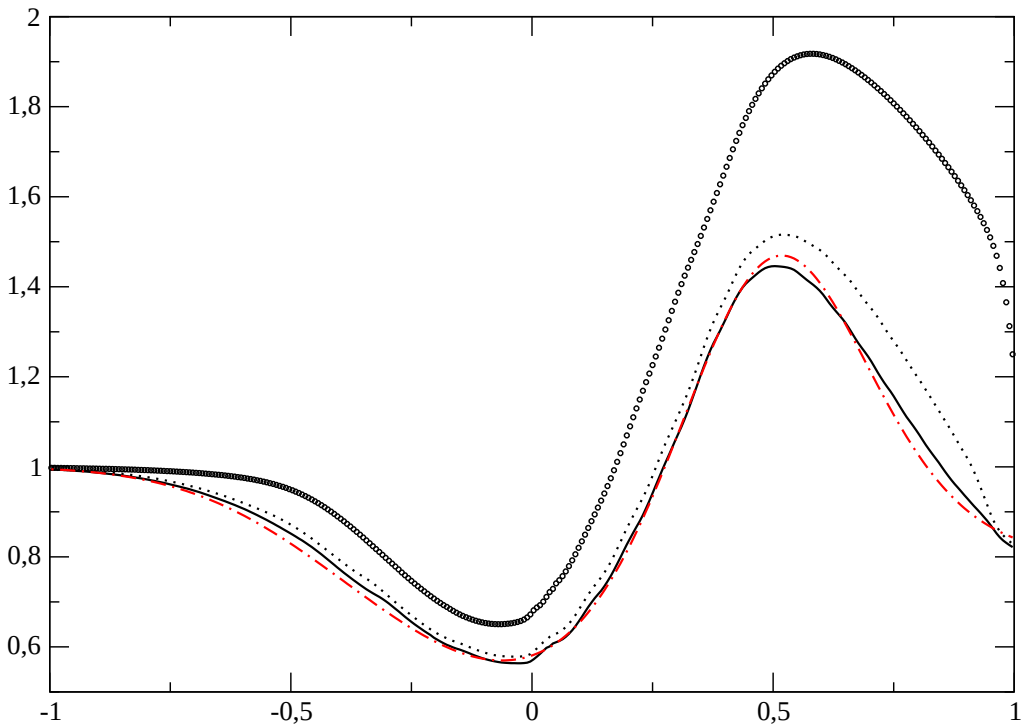

Figure 7: Sod test case, free transport: temperature at time 0.3, comparison between the exact solution (dot-dashed) and several LDVs with 30 points and the *moment correction method*: with first order interpolation ('o'), with 3 points-ENO (dotted), with 4 points-ENO (solid).

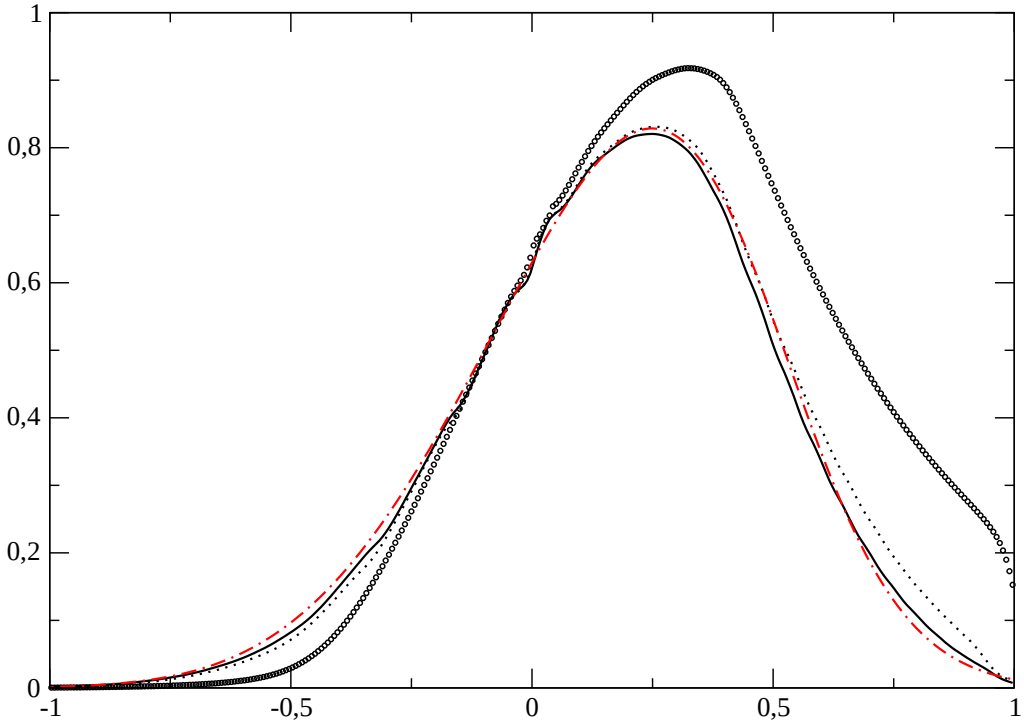

Figure 8: Sod test case, free transport: velocity at time 0.3, comparison between the exact solution (dot-dashed) and several LDVs with 30 points and the *moment correction method*: with first order interpolation ('o'), with 3 points-ENO (dotted), with 4 points-ENO (solid).

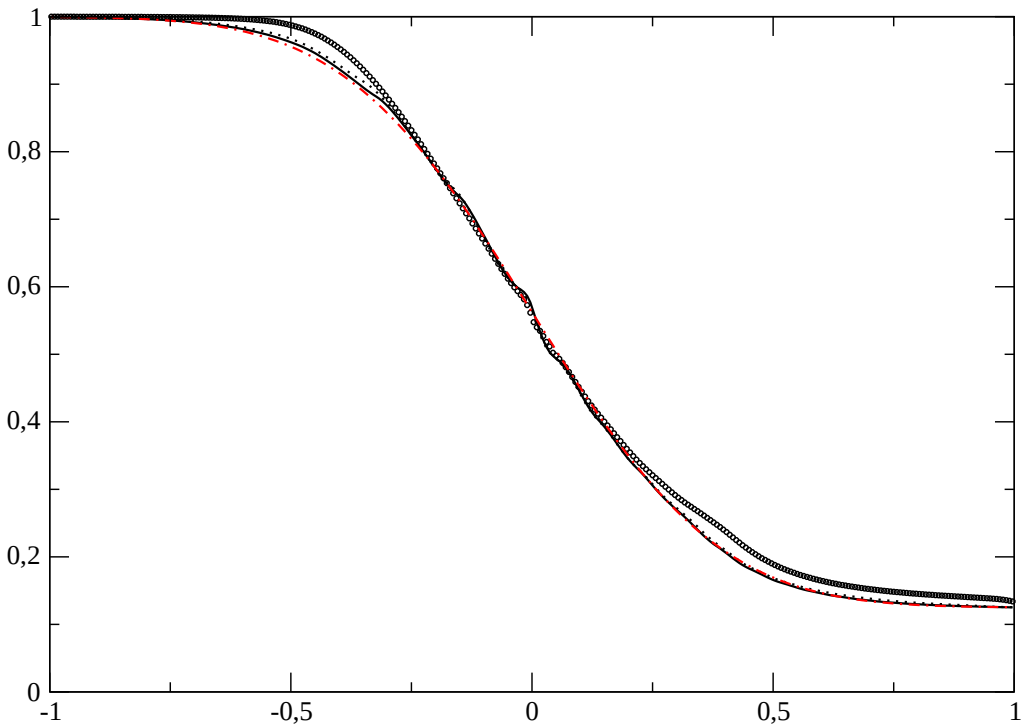

Figure 9: Sod test case, free transport: density at time 0.3, comparison between the exact solution (dot-dashed) and several LDVs with 30 points and the *moment correction method*: with first order interpolation ('o'), with 3 points-ENO (dotted), with 4 points-ENO (solid).

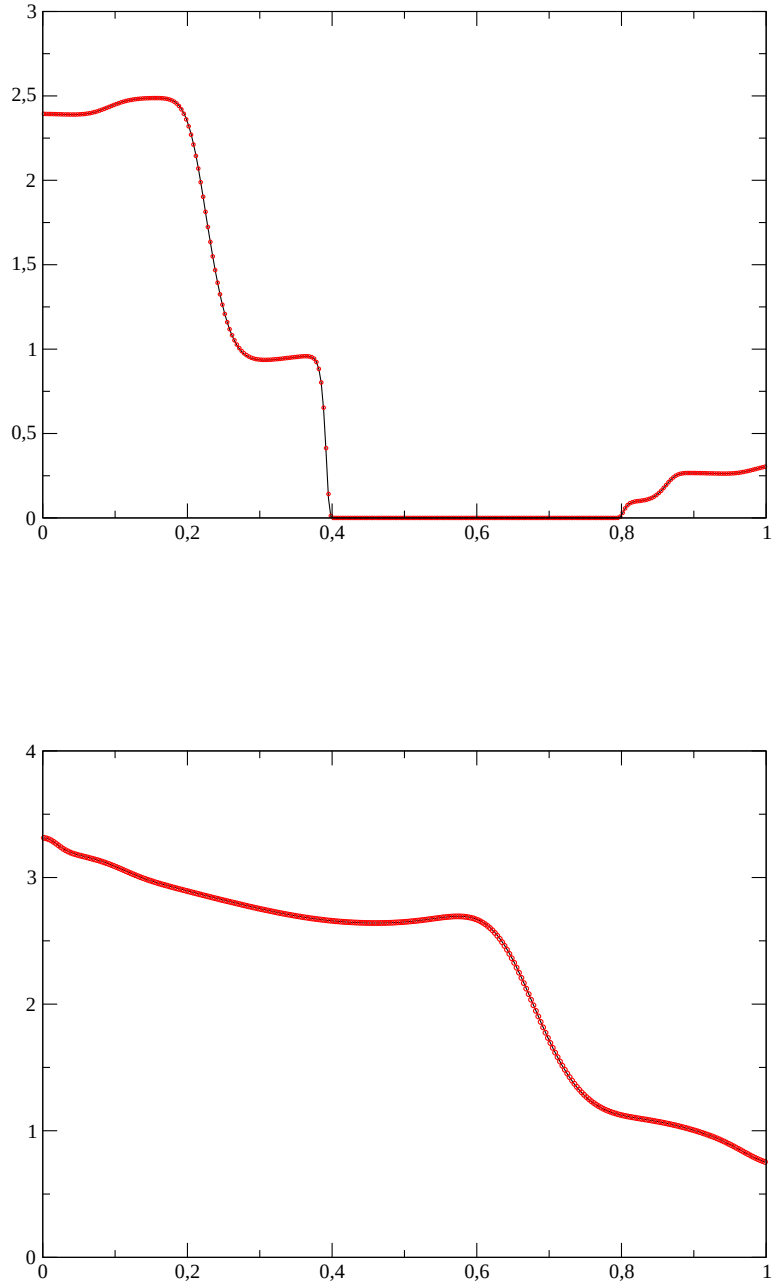

Figure 10: "Two interacting blast waves": temperature, before the shock at time 0.008 (top) and after the shock at time 0.05 (bottom). The solid line is the solution obtained with the LDV method (30 points), the dotted line is the solution computed with the DVM method (2 551 velocities).

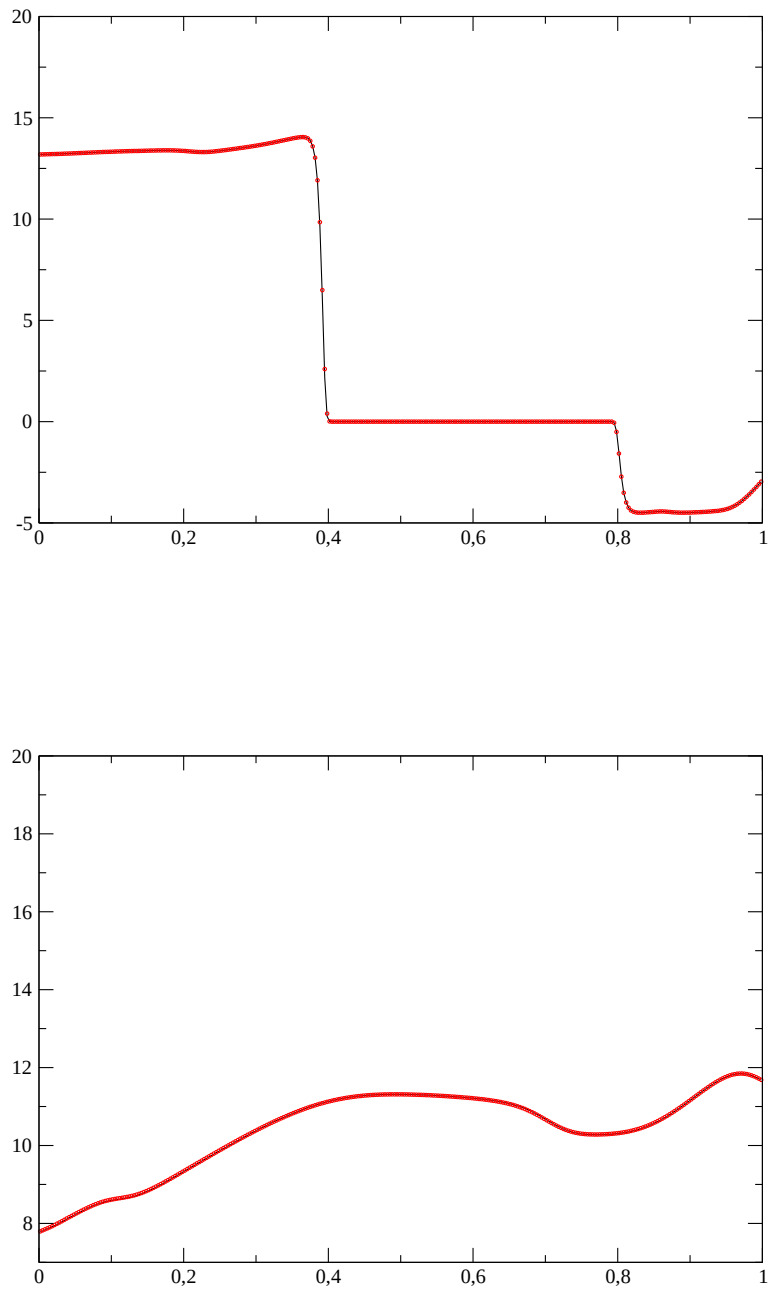

Figure 11: “Two interacting blast waves”: velocity (same as figure 10).

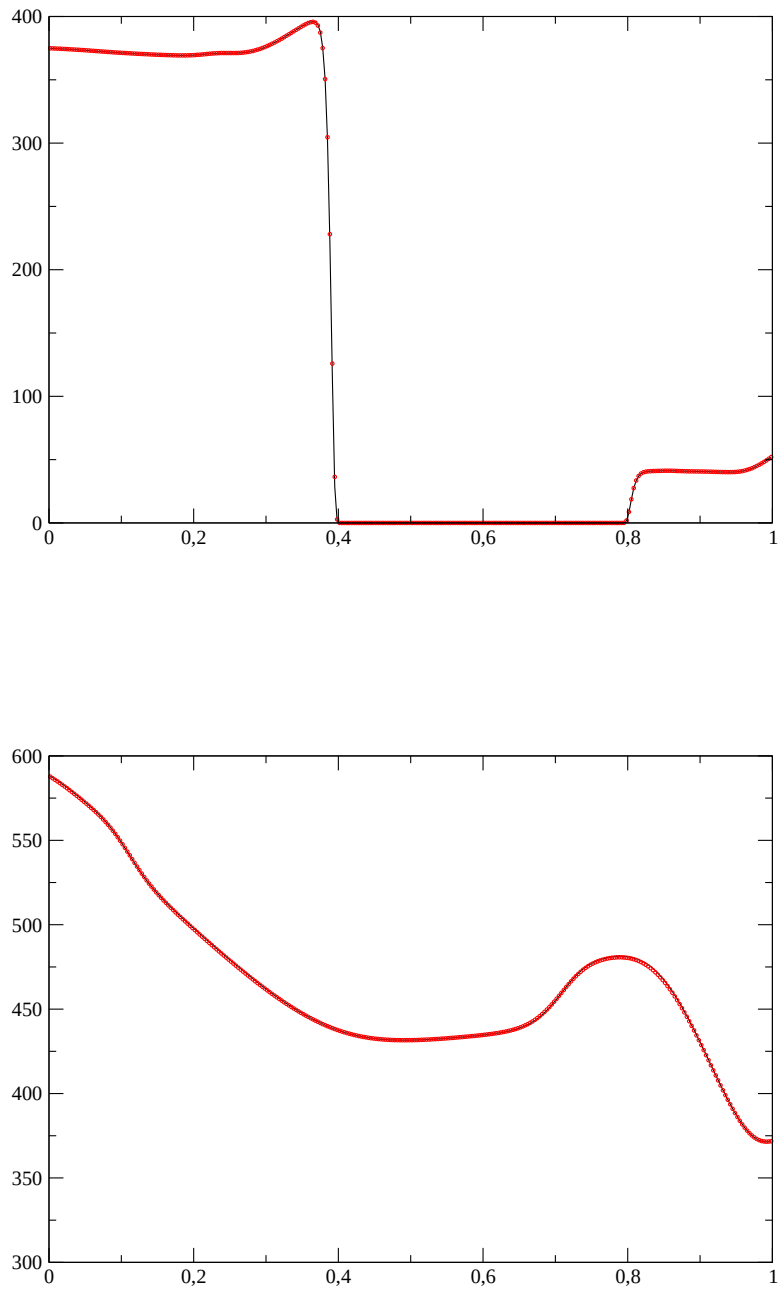

Figure 12: “Two interacting blast waves”: pressure (same as figure 10).

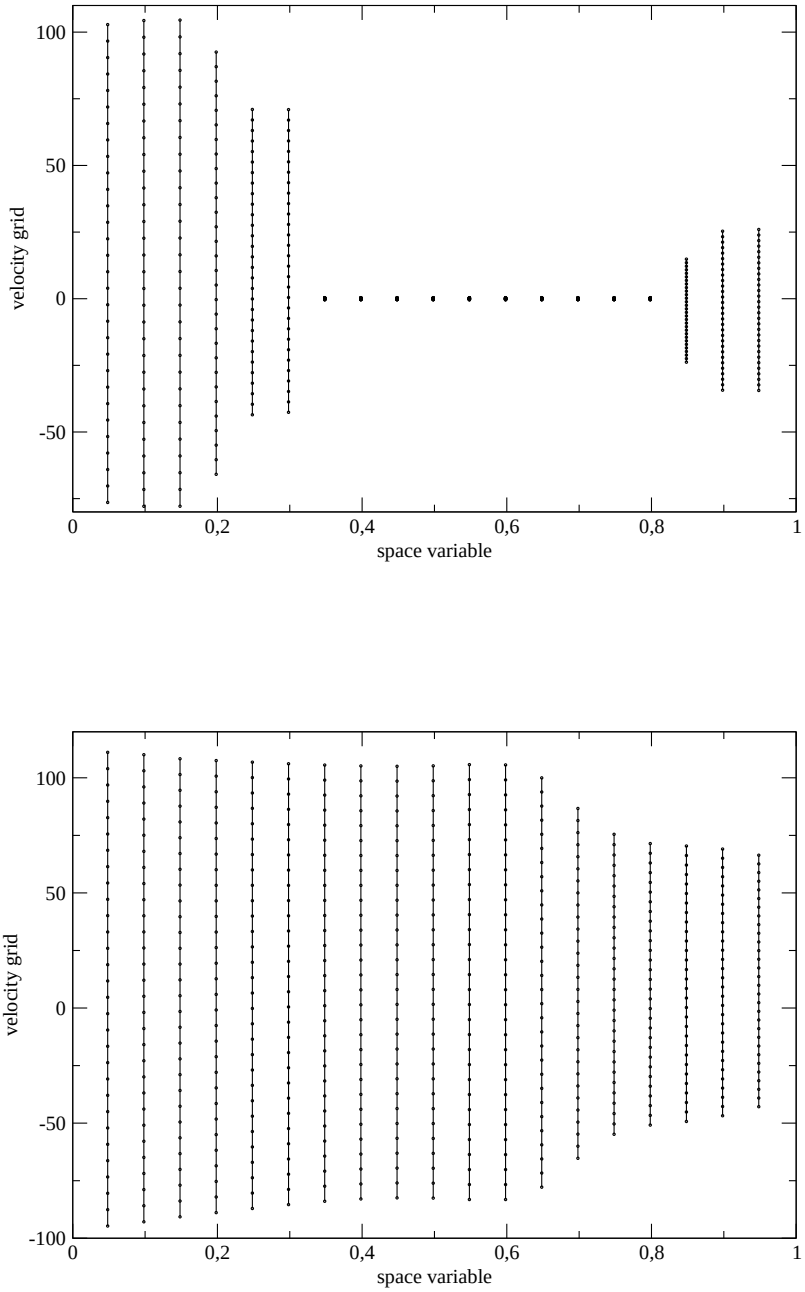

Figure 13: "Two interacting blast waves": some local velocity grids for different space positions, before the shock at time 0.008 (top) and after the shock at time 0.05 (bottom).

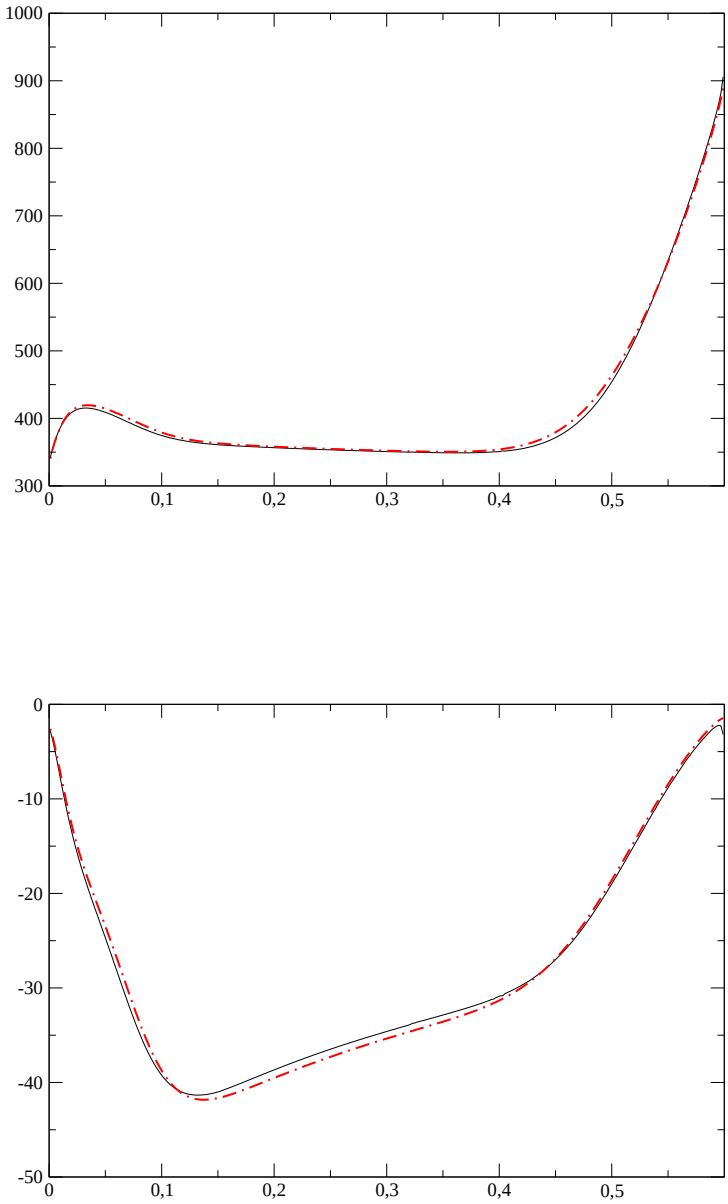

Figure 14: Heat transfer problem, transitional regime: temperature (top) and velocity (bottom) at time $1.3\,10^{-3}$, $\mathrm{Kn} = 10^{-2}$. The solid line is the solution given by the LDV method (30 velocities), the dot-dashed line is the DVM method (30 velocities).

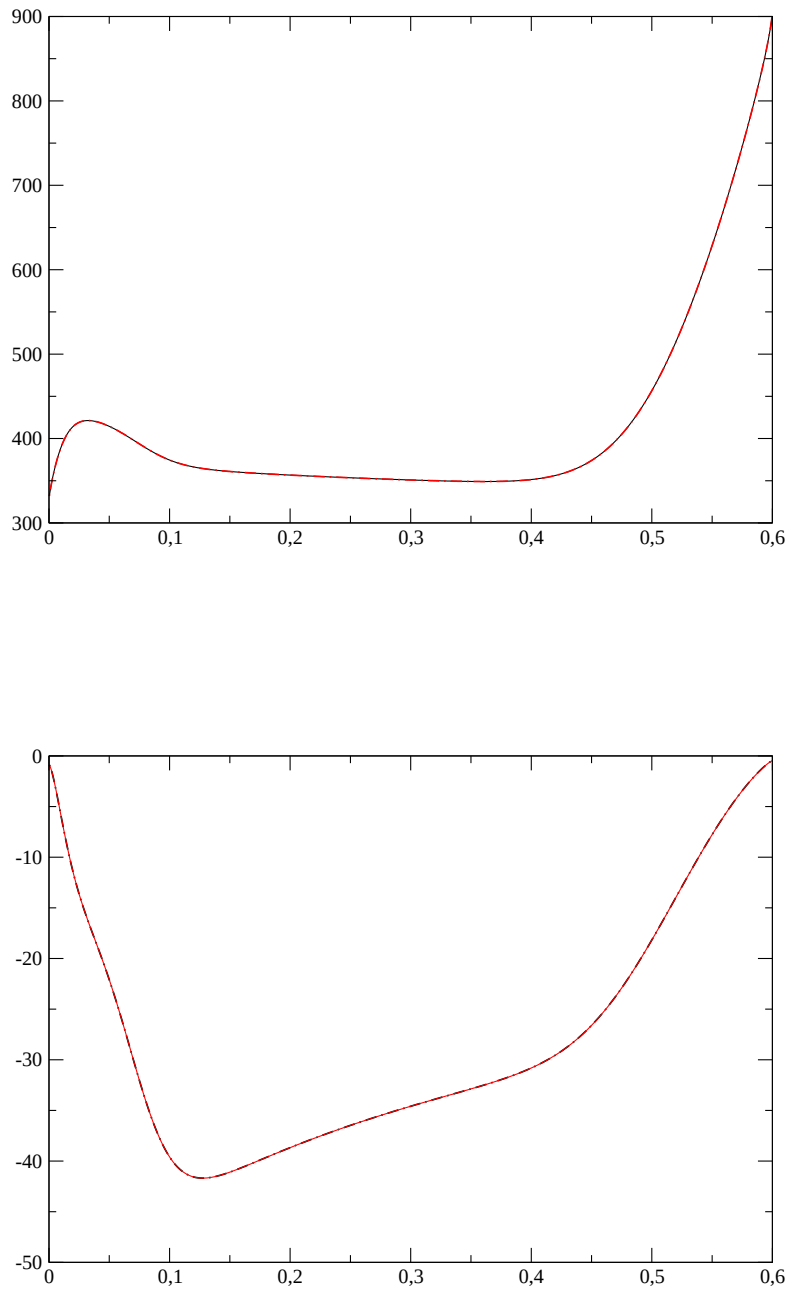

Figure 15: Heat transfer problem, transitional regime (test of the non symmetric local grid): temperature (top) and velocity (bottom) at time $1.3\,10^{-3}$, $\mathrm{Kn} = 10^{-2}$. The solid line is the solution given by the LDV method (30 velocities), the dot-dashed line is the DVM method (30 velocities).

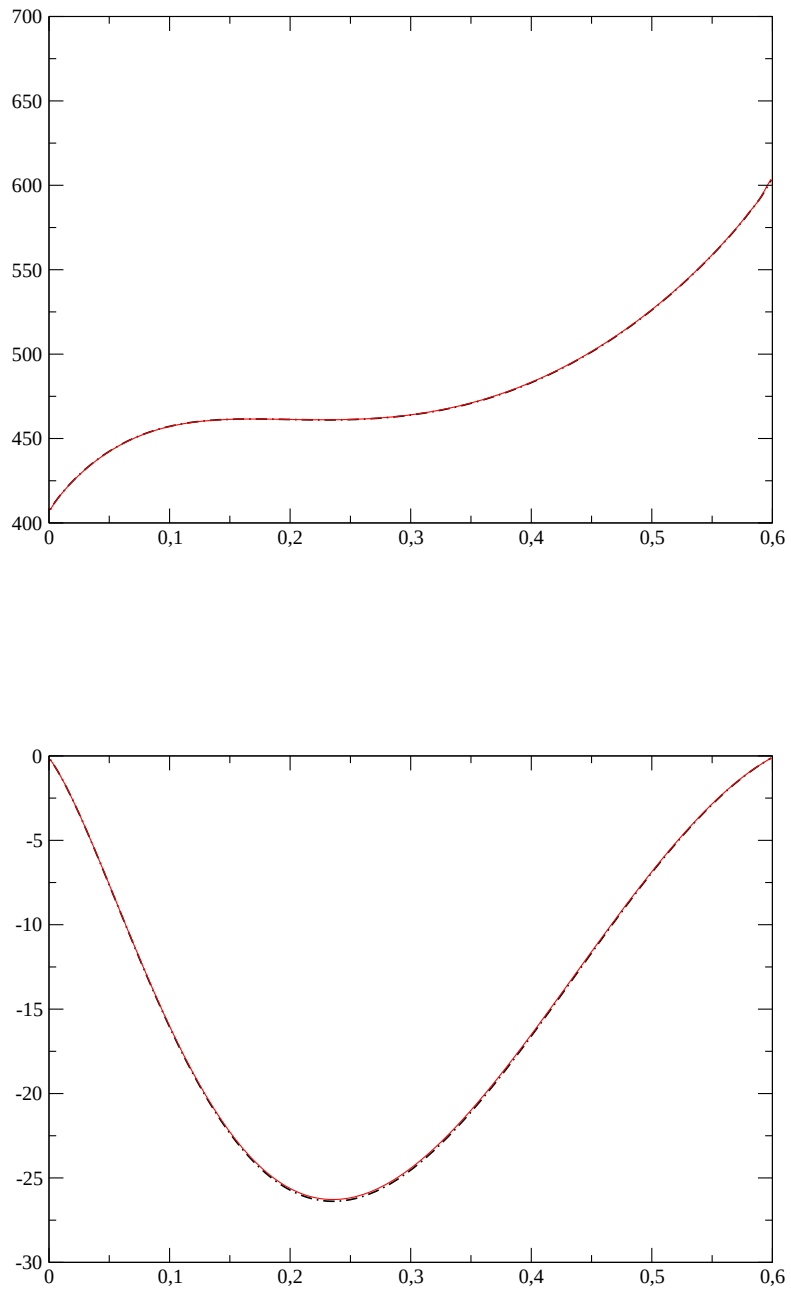

Figure 16: Heat transfer problem, rarefied regime: temperature (top) and velocity (bottom) at time $1.3\,10^{-3}$, Kn = 1. The solid line is the solution given by the LDV method (300 velocities, non symmetric local grids), the dot-dashed line is the DVM method (300 velocities).

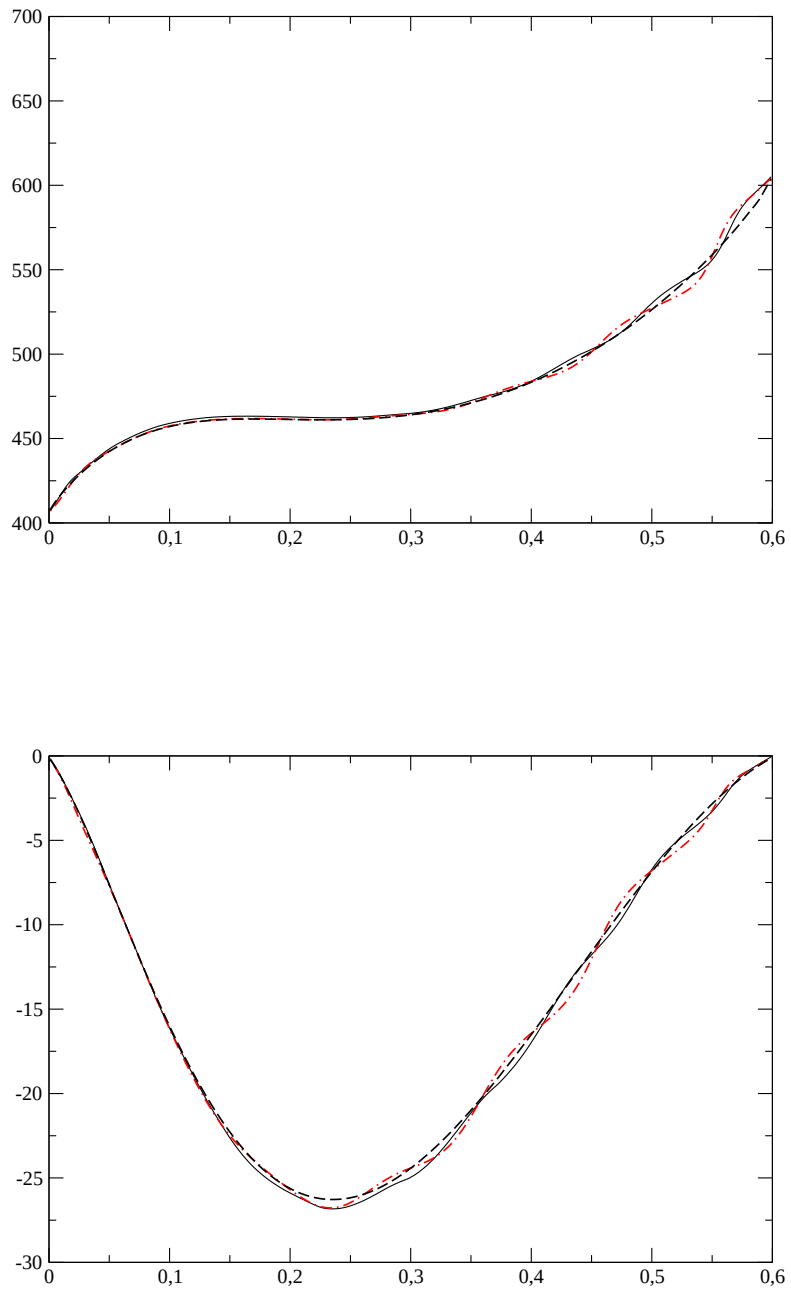

Figure 17: Heat transfer problem, rarefied regime: temperature (top) and velocity (bottom) at time $1.3\,10^{-3}$, Kn $= 1$. The solid line is the solution given by the LDV method (50 velocities, non symmetric local grids), the dot-dashed line is the DVM method (50 velocities), the dashed line is the DVM method with 300 velocities (reference solution).

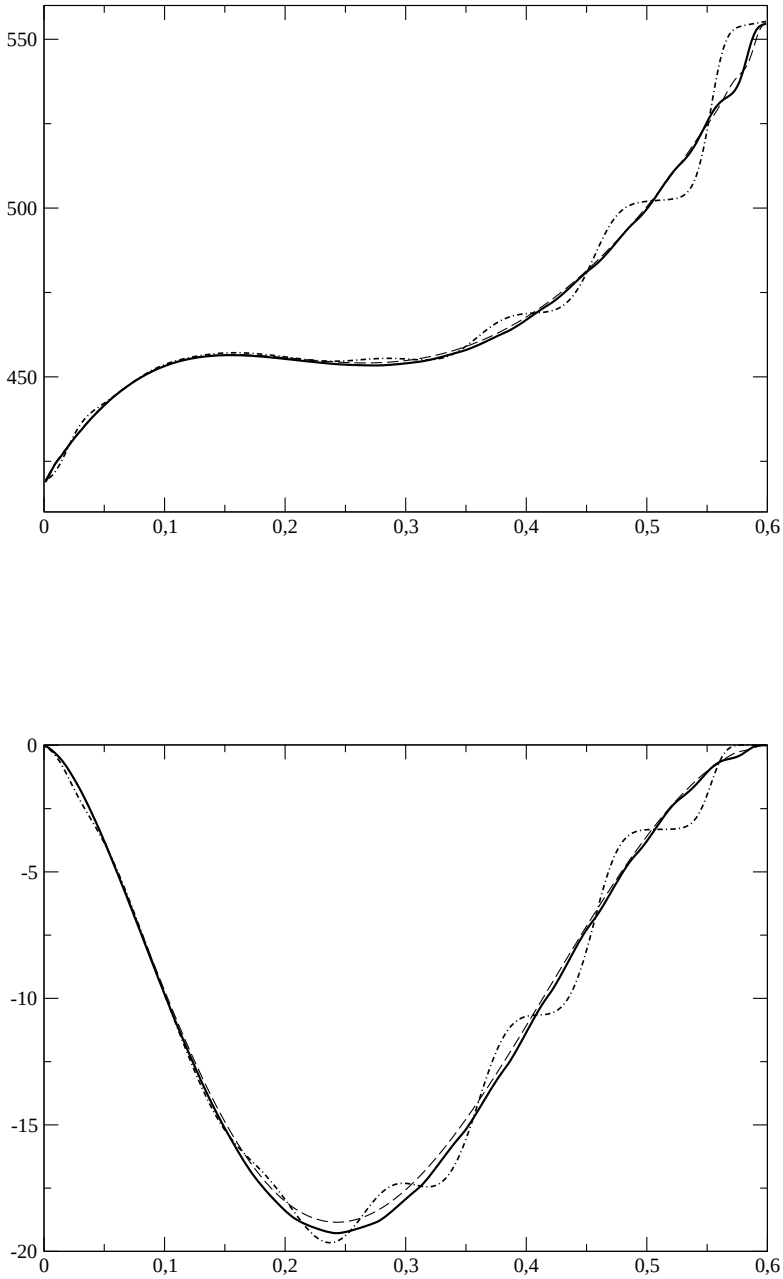

Figure 18: Heat transfer problem, rarefied regime: temperature (top) and velocity (bottom) at time $1.3\,10^{-3}$, Kn = 10. The solid line is the LDV method with 100 velocities, the dot-dashed line is the DVM method (100 velocities), the dashed line is the solution given by the DVM method (400 velocities, reference solution).

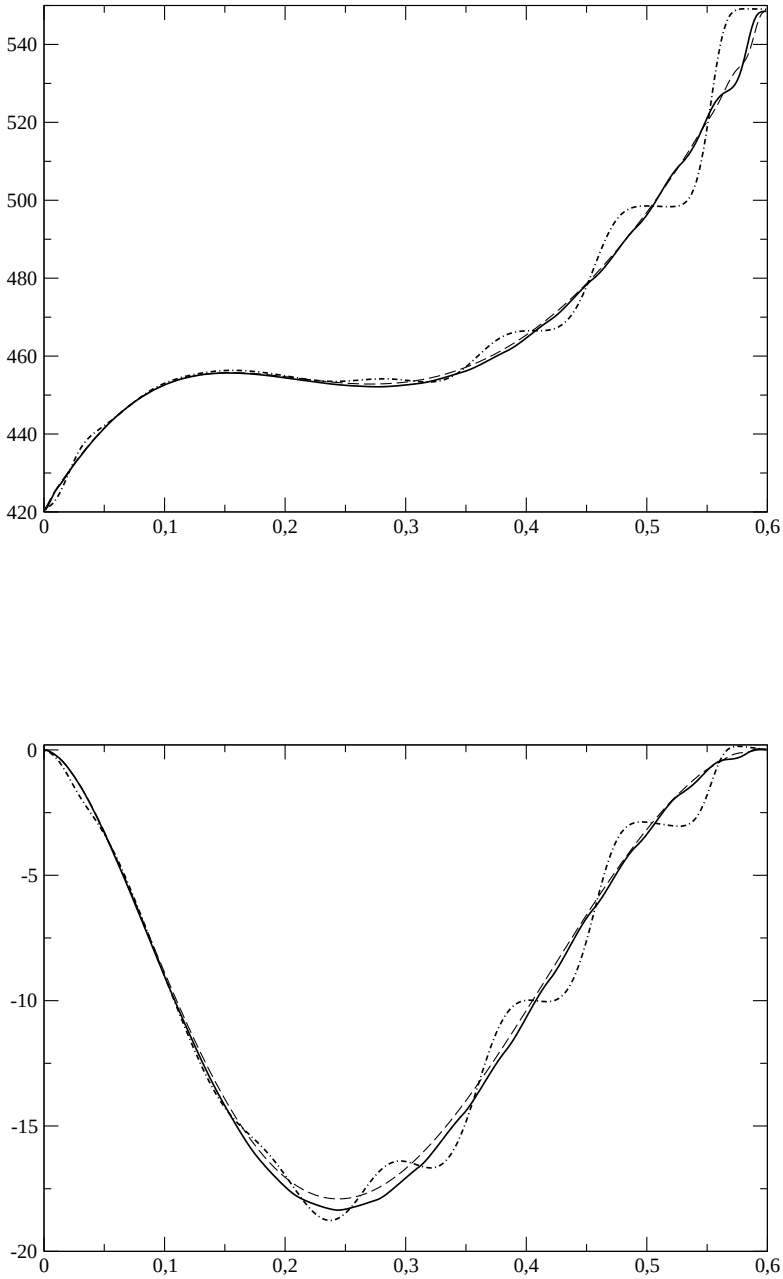

Figure 19: Heat transfer problem, rarefied regime: temperature (top) and velocity (bottom) at time $1.3\,10^{-3}$, Kn = 1000. The solid line is the LDV method with 100 velocities, the dot-dashed line is the DVM method (100 velocities), the dashed line is the solution given by the DVM method (400 velocities, reference solution).

	Sod	Blast waves	Heat transfer
DVM	0.344	949	64
LDV	5.136	20	14

Table 1: CPU time comparisons (in seconds) between the LDV and DVM methods