Modification of Godunov method for calculations of discontinuous two-temperature flows of low-temperature rare gas plasma

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Abstract. The paper presents the implementation of Godunov method for shocked flows of two-temperature rare gas plasma. An algorithm for cell edge convective fluxes calculation was developed. Algorithm is based on the solution of Riemann problem in rare gas plasma and includes accurate consideration of electrons adiabatic expansion. The theory uses the assumption that ionization and electrons-molecules collisional heat exchange rates are compatible with the characteristic time of the flow and can be neglected in Riemann problem solution.

1. Introduction
Godunov method belongs to the class of conservative methods and allows shock-capturing calculation of gasdynamics flows. According to the method, gasdynamics equations are integrated via the volume of computational grid cell and the fluxes of mass, momentum and energy on the cell surface are found from the solution of Riemann problem on the edge between the neighboring cells [1].

Originally, Godunov method was formulated for the ideal gas flows governed by Euler equations. But its algorithm for cell edges fluxes determination is also used for viscous flows [2].

In contrast to the neutral gas, weakly ionized gas contains ions and electrons besides the neutral molecules. During the collisions between electrons and heavy molecules (ions and neutrals), the energy exchange takes place, as well as the processes of ionization, molecules excitation etc. Due to large difference in electrons and molecules mass, typically, the equilibrium distributions in electrons velocities or molecules velocities come faster than the equilibrium between electrons and molecules temperatures [3,4].

Another mechanism of electrons-ions interaction is Coulomb potential. In considered flows, Debye length is about particles free path, so, concentrations of electrons and ions are equal in any point of the flow. Coulomb forces produce momentum exchange between electrons and ions. This interaction is non-collisional, so, the exchange happens immediately.

For example, when the gradient of electrons pressure occurs it affects the change of heavy particles velocity. Another example is a structure of shock wave in plasma [4]. The velocity of sound in electrons is significantly faster than that of molecular gas so, electrons shock wave should be ahead of the molecules shock wave. However, Coulomb forces do not allow the separation of electrons and molecules discontinuities.
The gap between electrons and molecules temperatures can be induced, for example, by the shock waves, by the electric current, by the light absorption in electrons, etc. The reverse process is the electrons-molecules collisional heat exchange which leads to temperatures equalization. The regions of two-temperature flow occur when the heat exchange speed is of the same order than the speed of flow gasdynamic processes.

2. The solution of Riemann problem in rare gas

Rare gases are very suitable object for two-temperature flow investigations. The list of plasmaphysic processes take place in rare gas plasma is limited. Typically, this list includes ionization, collisional heat exchange and radiation. The speed of these processes is not high and is comparable with characteristic times of typical supersonic low-temperature plasma flows. On the other hand, the molecule of rare gas consists of the single atom, which simplifies the Riemann problem solution.

The system of Governing equations of inviscid rare gas plasma looks as following:

\[
\frac{\partial U}{\partial t} + \nabla F - R = Q, \quad (1)
\]

\[
U = \left\{ \rho, \quad \rho V, \quad E + \frac{\rho V^2}{2}, \quad n_e, \quad E_e \right\}
\]

\[
F = \left\{ \rho V, \quad \rho VV + p_e, \quad \left( E + \frac{\rho V^2}{2} + p \right) V, \quad n_e V, \quad (E_e + p_e) V \right\}
\]

\[
R = \left\{ 0, \quad 0, \quad 0, \quad 0, \quad V \cdot \nabla p_e \right\}
\]

where \( U \) is the vector of gasdynamic functions, \( F \) is the vector of convective fluxes, vector \( Q \) contains the terms of radiation, ionization and collisional heat exchange between electrons and heavy particles, \( \rho \) is molecules density, \( V \) is plasma velocity, \( E_e, p_e, T_e, n_e \) are the energy, pressure, temperature and concentration of electrons, \( E \) is plasma energy, \( p \) is full pressure:

\[
p = p_h + p_e, \quad p_h = n_h k T_h, \quad p_e = n_e k T_e,
\]

where \( n_h, T_h \) are the concentration and temperature of heavy particles (ions and neutral molecules), \( n_h = \rho / m_h, \quad m_h \) is molecule mass.

Rare gas molecule consists of the single atom, therefore, rare gas heat capacity ratio is the same than that for the electrons \( \gamma = 5/3 \). Due to this fact, equation of state for rare gas plasma takes the form:

\[
E = \frac{3}{2} p_h + \frac{3}{2} p_e = \frac{3}{2} P.
\]

The term \( V \cdot \nabla p_e \) in vector \( R \) describes the energy transfer during the momentum exchange between electrons and ions.

Let us consider that the speed of the processes presented by vector \( Q \) in the system of equations (1) is low enough to neglect their effects on the formation of the self-similar distribution in the Riemann problem. In this case, system (1) takes the form:

\[
\frac{\partial U}{\partial t} + \nabla F = 0. \quad (3)
\]
The equations 1-3 in the system (3) supplemented by the equation of state (2) coincide with the Euler equations for ideal gas dynamics. The solution of Riemann problem for this case is well-known and can be found in [1].

Initially, gas is separated by the discontinuity plane into two regions with different gas conditions. After the flow starts, shock or rarefaction waves are forming in this regions and the initial discontinuity plane becomes the contact discontinuity.

The Riemann problem solution allows to obtain the distribution for $\rho$, $P$ and $V$. In addition, the distributions of $n_e$ and $T_e$ must be found. It can be done taking into account the following conditions. Firstly, in the absence of ionization, the ionization degree of the fluid volume is constant $n_e/n_n = \text{const}$. Secondly, the electrons-molecules heat exchange is also absent and electrons gas is governed by adiabatic equation $p_e/n_e^{5/3} = \text{const}$. Finally, the equations for $n_e$ and $T_e$ have the view:

$$n_e/n_{e0} = \rho/\rho_0, \quad p_e/p_{e0} = (n_e/n_{e0})^{5/3},$$

where subscript 0 means the initial gas conditions. According to the point position from the contact discontinuity, initial values are taken from the corresponding side from the initial discontinuity plane.

3. The discretization of the governing equations

Computational domain is divided by the grid into the cells with piecewise uniform distribution of gas parameters inside the cell. Godunov method uses the integral form of gasdynamic equations. When applied to the cell volume, integral form of system (3) looks as following:

$$\int_V \frac{\partial U}{\partial t} \, dVol + \int_S F dS - \int_R RdVol = 0,$$

where $Vol$ is cell volume, $S$ is cell surface. It is seen that gradient of the convective fluxes in the second term of (4) transformed into the surface integral. This transformation cannot be done with the $V \cdot \nabla p_e$ term of vector $R$. This feature does not allow to make (4) fully conservative.

Discrete form of time step for grid cell number $i$ looks like:

$$U_j(t + \Delta t) - U_j(t) = \frac{1}{Vol_i} \sum_j F(U_w) \cdot \vec{n}_j \cdot S_j + R_j,$$

where $U_w = \text{riemann}(U_i, U_j)$.

On the right hand of (5) there is a gasdynamic function time variation. On the left hand of (5) there is a sum of convective fluxes by the edges turned to the neighbouring cells denoted by the index $j$. In (5) $n_j$ is the edge normal vector, $S_j$ is edge surface, $U_w$ means the result of Riemann problem solution on the $(ij)$ edge.

Various ways of $V \cdot \nabla p_e$ spatial discretization can be found which are suitable for the continuous flows. But on the shock wave they cause the error in calculation of electrons temperature.

For illustration of this phenomenon the calculations of Riemann problem for the equations (3) were made using the following discretization of $V \cdot \nabla p_e$ term:

$$\int_V \frac{1}{Vol} V \cdot \nabla p_e \cdot dVol = V \int_S p_e \cdot dVol,$$
In figure 1 the comparison of calculated and theoretical profiles of electrons temperature is shown. The initial discontinuity was situated in $X = 0$. The profile of plasma density is also shown on figure 1 in order to illustrate the position of shock and rarefaction waves and contact discontinuity.

It is seen that the scheme is working good on the rarefaction wave (left side of figure 1) and predict incorrect electrons temperature after the shock wave. Calculations shows that this error reaches a considerable value of 12% at the shock wave Mach number $M = 2$.

![Figure 1](image)

Figure 1. The results of Riemann problem solution. The comparison of theoretical and calculated dimensionless electrons temperature distributions. The $V \cdot \nabla p_e$ term was discretized using equation (6).

The escape was found in the accurate accounting of the electron adiabatic expansion work. This algorithm will be described on the following example.

The work of the external forces during the electrons gas expansion has the following expression:

$$W_e = E_{e0} \left[ 1 - \left( \frac{n_{e1}}{n_{e0}} \right)^{3/2} \right], \quad E_e = \frac{3}{2} p_e \cdot Vol$$

where subscript 0 corresponds to start gas condition and 1 corresponds to finish condition, volume $Vol$ mean the volume occupied by the gas at start conditions. Introducing $W$ to the equations (3), the equation for electrons energy will take the form:

$$\frac{\partial}{\partial t} \left( \frac{3}{2} p_e \right) = -\nabla \left( \frac{3}{2} p_e V \right) + W_e,$$

where $W_e$ is the work of external forces.

Let us consider two neighbouring cells with the numbers $i$ and $j$ (figure 2). At the time $t_0$ the gas parameters in this cells were $p_{ei}, n_{ei}, p_{ej}, n_{ej}$, at the time $t_0+\Delta t$ this parameters became $p'_{ei}, n'_{ei}, p'_{ej}, n'_{ej}$. Beside them, $n'_{ei}$ and $n'_{ej}$ are known through the separate solution of $1 \cdot 4$ equations in system (5). The parameters on cells edge $V_{ij}, p_{ij}$ and $n_{ij}$ are found from the solution of the Riemann problem on the edge. Let the velocity have the right direction.
Figure 2. The scheme of gas evolution between two cells during the time step $\Delta t$. Left part illustrates the process of gas transition between the cells during the time between $t_0$ and $t_0 + \Delta t$. Arrow indicates the flow direction. Right part shows the cells condition at the time $t = t_0 + \Delta t$.

During the time $\Delta t$ the part of the gas lefted the cell $i$ for the cell $j$. The volume of this gas is $Vol_{ij} = S_{ij} V_{ij} \Delta t$. This gas made two transitions.

First transition was from the $p_{ei}$, $n_{ei}$ to $p_{eij}$, $n_{eij}$, its expansion work corresponds to $i$ cell and have the following expression:

$$W_{g_{i(t-\Delta t)}} = -\frac{3}{2} p_{ei} \cdot S_{ij} \cdot V_{ij} \cdot \Delta t \cdot \frac{n_{ei}}{n_{ei}} \left[ 1 - \left( \frac{n_{eij}}{n_{ei}} \right)^{\frac{2}{3}} \right],$$  

(8a)

Second transition was from $p_{eij}$, $n_{eij}$ to $p'_{eij}$, $n'_{eij}$, its expansion work corresponds to $j$ cell and have the following expression:

$$W_{ijt} = -\frac{3}{2} p_{eij} \cdot S_{ij} \cdot V_{ij} \cdot \Delta t \cdot \left[ 1 - \left( \frac{n'_{eij}}{n_{eij}} \right)^{\frac{2}{3}} \right],$$  

(8b)

The part of the initial gas which remained in cell $i$ after time $\Delta t$ can be found after the subtraction of gas parts lefted the cell through all edges. The remained gas made the transition from $p_{ei}$, $n_{ei}$ to $p'_{ei}$, $n'_{ei}$, its expansion works corresponds to $i$ cell and have the following expression:

$$W_i = -\frac{3}{2} p_{ei} \cdot \left[ Vol_i - \sum_j S_{ij} \cdot V_{ij} \cdot \frac{n_{ei}}{n_{ij}} \cdot \Delta t \right] \left[ 1 - \left( \frac{n'_{ei}}{n_{ei}} \right)^{\frac{2}{3}} \right],$$  

(8c)

Finally, the discrete form of electrons energy equation (7) takes the form.

$$\frac{3}{2} \frac{p_e(t + \Delta t) - p_e(t)}{\Delta t} = \frac{1}{Vol_i} \sum_j \left( \frac{3}{2} p_{eij} \cdot V_{ij} \cdot \bar{n}_{ij} \cdot S_{ij} - W_{g_{ij(t-\Delta t)}} - W_{ijt} \right) - W_i,$$  

(9)

The terms $W$ with $ij$ index in equation (9) and terms under the sum in (8c) are equal to zero when the edge velocity $V_{ij}$ is directed inside $i$ cell, the terms $W$ with $ji$ index in equation (9) are equal to zero when the edge velocity is directed outside $i$ cell.

The calculations of the Riemann problem using the discretization (9) are presented on figure 3. It demonstrates good resolution of all types of discontinuities.
4. Conclusion
The modification of Godunov method was developed for the calculations of two-temperature supersonic flow of low-temperature rare gas plasma.

An algorithm of the Riemann problem solution in rare gas plasma was presented.

The presence of special term $V \cdot \nabla p_e$ in the equation for electrons energy does not allow conservative form of the gasdynamic equations. The original algorithm for calculation of electrons adiabatic expansion was formulated which allows to approximate $V \cdot \nabla p_e$ term.

The developed method demonstrates correct resolution of gasdynamics discontinuities and allows shock-capturing calculations of the rare gas plasma supersonic flows.

References
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