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CONSERVATIVE BOUNDARY CONDITIONS FOR THREE-DIMENSIONAL GAS DYNAMIC PROBLEMS

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1. Introduction

At present in computational gas dynamics [1] there are well- /3*
developed methods based on isolation of discontinuities, making
use of calculation grids adapted to the boundary. Such approach
[2-3] affords high accuracy, although the computerized construc-
tion of a difference grid involves major software difficulties,
especially in the case of a moving boundary and other nonsta-
tionary processes.

The tasks of contemporary engineering gas dynamics are dis-
tinguished by great diversity of geometries and boundary condi-
tions, and even an approximate solution often enables an assess-
ment as to the prospects of a gas dynamics apparatus under
development. There also exist a multiplicity of problems in
which the gas flow itself plays a subordinate role in relation
to the other dominant physical processes for which only extremely
crude models are available (physical gas dynamics). In these
applications, it seems advisable to expect the following demands
of the computer algorithm:

1. A unified approach to the solving of different types of
problem, with easy enlargement of the physical content.

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*Numbers in the margin indicate pagination in the original text.

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2. Easy operation of the program, not requiring a highly qualified computer mathematics user.

3. Satisfactory practical precision at relatively short computer run time.

It is difficult to satisfy requirements 1-3 with traditional numerical methods. The methods best suited to this are a start-to-finish calculation [1], which has been a stimulus to the development of the latter. The use of boundary-nonadapted regular grids and explicit schemes enables a simplification of the algorithm, an automated running of the program, and consequently an appreciable enlargement of the range of users.

Various authors have elaborated this method for the two-dimensional case [4-9]. The chief shortcomings of the methods described in [4-6] are the nonconservativeness, the nonhomogeneity and the cumbersome formulas in the boundary compartments of the grid, which do not allow a generalization of these methods to the case of an arbitrarily moving, curvilinear boundary in a complex three-dimensional configuration. This complicated algorithmic procedure has another shortcoming--the boundary conditions are difficult to realize on nonuniform rectangular grids. The methods advocated in [5,6] are based on direct approximation of the derivatives at the node next to the boundary, which results in a large error at nodes with a heavily nonuniform pattern, complicates the software realization, and inadmissibly limits the time interval of explicit layouts. These shortcomings /4 led the author [5] to the conclusion that nonadapted grids have few prospective applications.

However, the above does not apply to the scheme [7-9] derived on nonadapted grids by the integro-interpolation method (IIM) [10]. Use of the IIM enabled simple difference formulas for the

two-dimensional case, assuring conservativeness of the start-to-finish calculation of the flow parameters in the interior and boundary compartments even for moving boundaries of complicated shape. Joining small compartments to the neighboring ones provides adequate stability of the difference scheme.

The present work generalizes the approach developed in [7-9] to the case of three-dimensional solids of complicated shape.

2. The Numerical Method

Let us consider the equations describing multidimensional flow of a nonviscous gas in Eulerian variables:

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + div\,(\rho\,\vec{W}) = 0 \\[2mm] \dfrac{\partial \rho \vec{W}}{\partial t} + Div(\rho\,\vec{W}\cdot\vec{W}) + grad\,P = 0 \\[2mm] \dfrac{\partial \rho E}{\partial t} + div\,(\rho E\,\vec{W}) + div\,(P\cdot\vec{W}) = 0 \\[2mm] P = P\,(\rho,\varepsilon) \end{cases} \qquad (1)$$

or the equation for the total energy E can be replaced by the equation for the internal energy ε:

$$\frac{\partial \rho \varepsilon}{\partial t} + div\,(\rho\varepsilon\,\vec{W}) + P\cdot div\,\vec{W} = 0$$

where $\vec{W} = (W^1, W^2, W^3)$ is the velocity, P the pressure, ρ the density. System (1) is solved in the region G with boundary $\Gamma = \Gamma^\ell$ (Fig. 1), where Γ^ℓ can be of three kinds: 1) the entry boundary Γ^ℓ_{bx}, where conditions of the first kind are usually set; 2) the exit boundary Γ^ℓ_{bux}, where we shall set the condition

of vanishing of the normal derivatives of the gas dynamic quantities; 3) the solid wall Γ_T^ℓ or planes of symmetry Γ_c^ℓ, where we have the condition of no flow-through:

$$(\vec{W} \cdot \vec{n}) = 0 \qquad (2)$$

where $\vec{n}$ is the normal to the wall.

The surface of the solid is given by the function F:

$F(x,y,z) > 0$, point (x,y,z) lies outside the solid
$F(x,y,z) = 0$, point (x,y,z) is on the solid $\qquad (3)$
$F(x,y,z) < 0$, point (x,y,z) lies inside the solid.

The boundaries Γ_{bx}^ℓ, $\Gamma_{b\mu x}^\ell$ and Γ_c^ℓ are situated in the coordinate planes. We shall complement the region G to produce a coordinate rectangle by introducing the region G_T, corresponding to the solid. We cover the rectangle $G + G_T$ with a nonuniform rectangular grid, producing three types of compartment:

a) a full compartment, entirely situated in the gas (inside region G)

b) a partial compartment, intersected by the boundary of the solid (in the calculations of the field of flow only that portion occupied by gas is involved)

c) an empty compartment, entirely situated in the solid (inside region G_T - hereafter omitted from the calculations, and such compartments are totally absent from the specially organized computer memory files.

Furthermore, we introduce a layer of imaginary compartments G_ϕ along $\Gamma_{b\mu x}^\ell$, Γ_c^ℓ. After this, the grid is complemented to a

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rectangle by the region $G_{\text{доп}}$, the compartments of which are equivalent to empty ones. The center of each compartment corresponds to the index $i = (i_1, i_2, i_3)$. Hereafter, we shall omit from the variables the indexes of directions on which no difference operations are performed. For the compartment of type a,b (Fig. 2), we introduce the following geometrical parameters: $S_{\pm}^{m} = S_{1m \pm \frac{1}{2}}$ - surfaces of the side faces of the compartment i open to passage of gas in the direction $i_m = 1,2,3$; V_i - the volume of the compartment occupied by gas. The proposed technique can be developed on the basis of any given explicit divergent (flow) method of start-to-finish calculation. The results of the two-dimensional calculations [7-9] revealed that the FLIC method [11] is a convenient reference point, in which the values of all the gas dynamic variables $\varphi = [\rho, \rho \vec{W}, \rho E]$ are adjusted to the centers of the compartments.

This method is based on consecutive calculation of the physical processes - transition from the n-th to the (n+1)-th time layer is done in a two-stage (in the case of moving boundaries, three-stage) scheme with a summary approximation [10].

In the first stage, only the action of pressure forces with transport processes held in abeyance is considered. To smooth out pulsations behind the shock wave front, it is possible to introduce an artificial viscosity. We shall assume such viscosity by analogy with the second physical [viscosity?] [9]:

$$q \sim div\,\vec{W}$$

in contrast with [4,5,7,8] this is added to the gas pressure [3]:

$$p' = p + q$$

which simplifies the algorithm and improves the equalization of

pulsations in the multidimensional case (hereafter we shall write the combined pressure without the prime). Let us apply the procedure described in [7] to a compartment or test volume. We integrate system (1) throughout the volume of the compartment i and replace the time derivative with its difference analog:

$$
\begin{cases}
\dfrac{^1(\rho\vec{W}) - {}^0(\rho\vec{W})}{\tau} + \displaystyle\int_{V_i} \operatorname{grad} P \, dV = 0 \\[3mm]
\dfrac{^1(\rho\varepsilon) - {}^0(\rho\varepsilon)}{\tau} + \displaystyle\int_{V_i} P \cdot \operatorname{div} \vec{W} \, dV = 0
\end{cases}
\tag{4}
$$

The index 0 refers to the value of the variables in the n-th layer, 1 after the first stage, 2 after the second. Using the familiar formulas of vector analysis, we change the volume integrals in (4) into surface integrals:

$$
\begin{aligned}
{}^1(\rho\vec{W}) &= {}^0(\rho W) + -\tau \int_S P \cdot d\vec{S} \\
{}^1(\rho\varepsilon) &= {}^0(\rho\varepsilon) - \tau \cdot P \cdot \int_S \vec{W} \cdot d\vec{S}
\end{aligned}
\tag{5}
$$

On the side faces of the compartment open to the passage of gas all the quantities shall be approximated by the half-sum of the values in the corresponding compartments. It follows from (2) that $(\vec{w} \cdot d\vec{s}) = 0$ on the solid wall; therefore, the wall in (5) provides a zero contribution to the energy integral. Provided that the spacing of the grid is much less than the radius of curvature of the solid, we have from (2):

$$
\frac{\partial P}{\partial n} = 0
\tag{6}
$$

which lets us regard the pressure on the wall in (5) as equal to the pressure at the center of the compartment.

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As a result, we obtain approximation formulas for the first stage:

$$
\begin{cases}
({}^{1}W^{m} - {}^{0}W^{m})\varrho V = -t\tfrac{1}{2}(S^{m}_{\cdot}\cdot P_{x_m} + \\
\qquad\qquad + S^{m}_{-1}\cdot P_{\bar{x}_m}) \\
({}^{1}\mathcal{E} - {}^{0}\mathcal{E})\varrho V = -\dot{P}\cdot t \cdot \sum_{m=1}^{3}(S^{m}\cdot{}^{t}\vec{W}_{+\frac{1}{2}} - \\
\qquad - S^{m}_{-1}\cdot{}^{t}\vec{W}_{-\frac{1}{2}}) \\
\qquad {}^{t}\vec{W} = 0.5\cdot({}^{0}\vec{W} + {}^{1}\vec{W}) \\
\qquad W^{m}_{+\frac{1}{2}} = 0.5\cdot(W^{m} + W^{m}_{+1})
\end{cases}
$$

In the second stage, convective transport is factored in. The procedure of obtaining the difference formulas is similar to the first stage procedure. In this case we use a "scheme with wind-ward differences". This scheme conveys rather precisely the characteristic physical features of the flow, i.e., it possesses the attribute of transportiveness. For the second stage, we get the following difference formulas:

where

$$
({}^{2}\varphi - {}^{1}\varphi)\cdot V = -t\sum_{m=1}^{3}(\Delta^{m}\varphi - \Delta^{m}_{-1}\varphi)
$$

$$
\Delta^{m}\varphi = 0.5\cdot S^{m}(({}^{1}W^{m}_{+\frac{1}{2}} + |{}^{1}W^{m}_{+\frac{1}{2}}|)\cdot{}^{1}\varphi +
$$
$$
+ ({}^{1}W^{m}_{+\frac{1}{2}} - |{}^{1}W^{m}_{+\frac{1}{2}}|)\cdot{}^{1}\varphi_{+\frac{1}{2}})
$$

For the first-order explicit method described, the Courant condition is a criterion of stability (for more details cf. [12]). To avoid excessively severe limitations on the time interval, each small partial compartment (with volume less than 20-30% of a full compartment) is joined to its neighbor.

3. The Software Realization

The program AEOL-3 is written in the language FORTRAN, making use of the conventions of the OLYMPUS system [13,14] and being an expanded version of the AEOL-2 application program package for the three-dimensional case. The structure of the program and the interplay between its modules conform to the general layout of the AEOL package. The programming does not employ any specific features of a particular FORTRAN version, and therefore can be used in virtually any computer of sufficient capacity. The package was developed in the BESM-6, but is run in the YeS-1045. The computer run time is relatively short: establishing a stationary flow past a complicated three-dimensional solid on a grid of 22,000 compartments (working storage around 1 MGB) takes less than 3 hours of machine time of the YeS-1045. Only the construction of the modules CURVE and CUBE differ significantly from the two-dimensional version AEOL-2. These perform the computation of the geometrical parameters of the partial compartments. If the boundary is immobile, the subprograms are called up only once at the start of the program. CURVE effects a scanning of the compartments of the grid, the geometrical situation in each partial compartment being solved independently, which also enables a uniformity of solving different types of problem. The CURVE and CUBE modules employ a function for specification of the shape of the solid (3), formulated as a subprogram - the function $FCUR(x,y,z)$. The lengths of the edges of a partial compartment are determined by solving the equation $FCUR(x,y,z) = 0$ on the corresponding edge by the method of dividing the segment into halves. If the boundary of the solid passes exactly through one of the vertexes of the compartment, we shift the boundary a slight distance away from the vertex (usually less than 0.1%) for uniformity of the algorithm.

To simplify the finding of the area of a particular side face of a partial compartment, the line of intersection of the face with the boundary of the solid is approximated by a straight line segment. If (q_1, q_2) and (b_1, b_2) are the pairs of lengths of opposite edges of the same face, it is easy to obtain a homogeneous formula:

$$S = 0.5 \cdot (a_1 + a_2) \cdot (\ell_1 + \ell_2) - min(a_1, a_2) \cdot min(\ell_1, \ell_2)$$

The subprogram CUBE calculates the volume of the portion of a compartment with a lesser number of vertexes, which is subtracted as needed from the volume of the corresponding full compartment. Through geometrical manipulations (rotation, mirror and central symmetry, parallel translation), the spatial configuration is reduced to one of the standards. Depending on the type of configuration, we calculate the volume by a particular approximation formula, and if the situation is nonstandard, the program is automatically halted and an error notification is sent. (A nonstandard situation is easily corrected by modifying the grid, cf. Fig. 3f.) The version being used at a given time provides five standard configurations (Fig. 3a-e), which enable analysis of practically all configurations.

The described standardization of cases of intersection of a three-dimensional compartment by the solid substantially simplifies the program logic, reduces the run time, enables a unification of the program complex and facilitates its mastery by the user having no special training. The user is only expected to specify the shape of the solid in the FCUR function program.

On the foundation of a unified geometrical data base, two subsystems have been created in the AEOL-3 program complex:

a) calculation of the hydrodynamics, b) visualization on display screen of the shape of an intricate object by lighting up the lines of intersection of the surface described by the function FCUR(x,y,z) with the planes of the grid. This program appreciably simplifies the shape adjustment process.

4. Test Computations

To test the proposed procedure of start-to-finish calculation, we shall solve the problem of a supersonic gas flow past a particular standard solid on various grids and shall compare the results with standard tables. A sphere on a uniform Cartesian rectangular grid is a solid of practically arbitrary shape (Fig. 3g). Therefore, we examine the streaming of a gas flow with parameters $M_\infty = 2$, $\gamma = 1.4$, $P_\infty = \rho_\infty = 1$ around a unit sphere on grids 21 x 24 x 32 and 18 x 18 x 24 with constant spatial intervals $h_x = h_y = 0.103$ and 0.164, $h_z = 0.0594$ and 0.095, respectively. On the first grid, in the entire field of flow outside the zone of discontinuity the differences of the pressure and density from the tabulated data [15] did not exceed 3% and 6%, while the drag was in agreement within 1.5%. /10

Figure 4 shows graphs of the pressure distribution along radii making angles $\omega = 0°$, $60°$, $90°$ with the direction of the flow; Fig. 5 shows the pressure distribution along the solid. The curves obtained from a calculation on a detailed grid are indicated by 1, those from a more coarse grid by 2. Figure 6 and 7 show the corresponding density profiles. It is evident from the graphs that the agreement of the pressure and density fields on both grids is perfectly satisfactory. Comparison of the calculation results on the two grids demonstrates the convergence of the method as the grid becomes more fine. It should be pointed out that an accuracy better than 1% should not be

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expected for realistic grids in our method, since the parameters within the grid compartment are assumed to be constant. In order to clarify the role of the mutual arrangement of the solid and the grid, the sphere flow problem was again solved on a grid of 24 x 24 x 32, but with the center of the sphere shifted $0.5 \cdot h_z$ along the flow. As compared to the former case, the difference in pressure field was less than 1%, but the difference in the drag force remained within 1.5%. This result is a dramatic illustration of the reality of the above-mentioned accuracy limit level of 1%.

In problems of experimental design the foremost consideration is the distribution of pressure along an object and the aerodynamic coefficients, as well as the nature of their change as the shape of the object is varied. Analysis of the test calculations reveals that the developed technique, realized in the AEOL-3 program complex, is able to solve such problems on extremely coarse grids with tolerable precision.

5. Calculation of the Flow Around a Three-Dimensional Object of Intricate Shape

Let us consider the problem of a gas flow with parameters $M_\infty = 3.5$, $p_\infty = \rho_\infty = 1$, $\gamma = 1.4$ around an obtuse object. The general appearance of the object in Fig. 8a is shown by the lines of intersection of the object's surface with the coordinate planes. Figure 8b and 8c show the field of pressure in the plane of symmetry and in the horizontal meridional section. About the periphery of the graph are also shown the grid plane markings, illustrating the distribution of the intervals. It should be noted that, despite the small dimensions of the recess in the meridional plane as compared to the grid interval (Fig. 8c), the method provides an excellent resolution of the secondary shock. The lift force at such object is negative, which was /11

found in the calculations and is entirely explained by the presence of the secondary shock, which increases the pressure in the upper half.

The calculations were done on grids with different spatial intervals, the difference in the vertical and horizontal aerodynamic coefficients not exceeding 2%. A standard analysis was done on a grid of 15 x 35 x 34 (22,000 compartments) and took less than 3 hours in the YeS-1045.

6. Conclusion

The paper describes a conservative method of unified computation of three-dimensional flow in the region of a complex shape. The accuracy suitable for practical purposes, the relatively modest computer run time, and the simple structure of the program complex render it a useful tool in the study of engineering gas dynamic problems.

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Fig. 1

Fig. 2

a)

b)

c)

d)

Fig. 3

e)

f)

$\overrightarrow{W}$
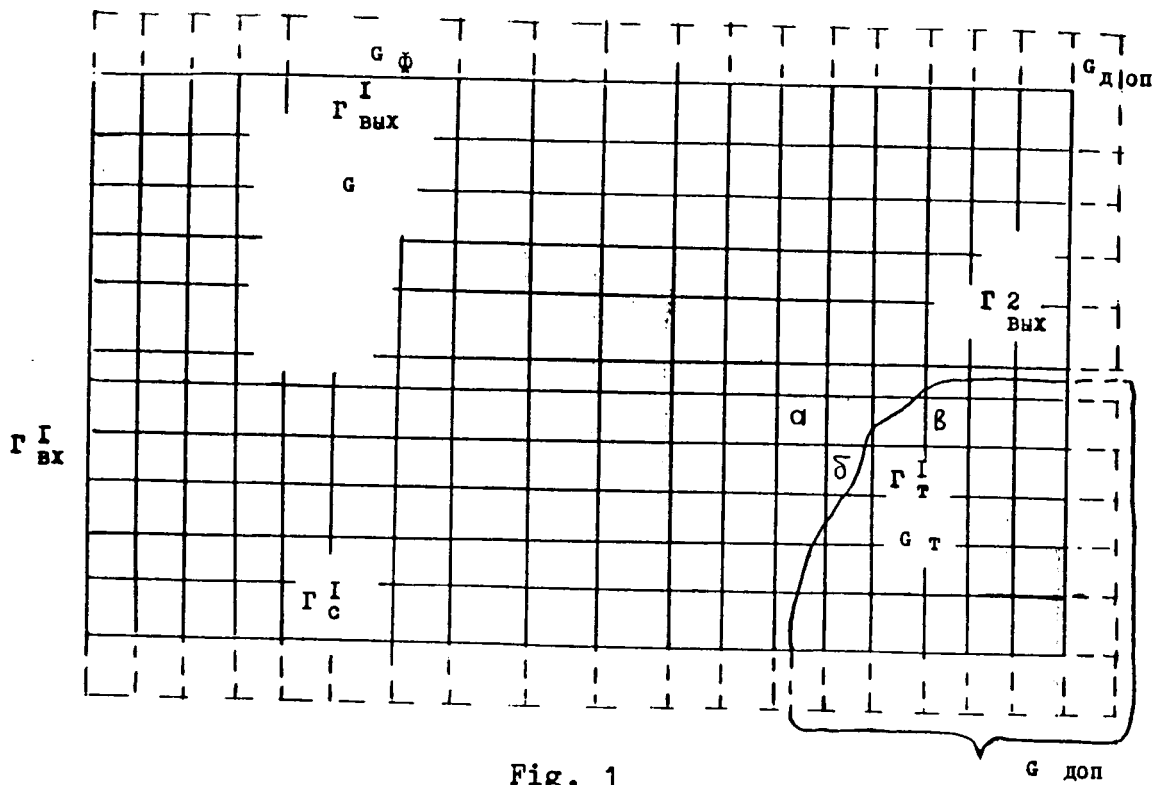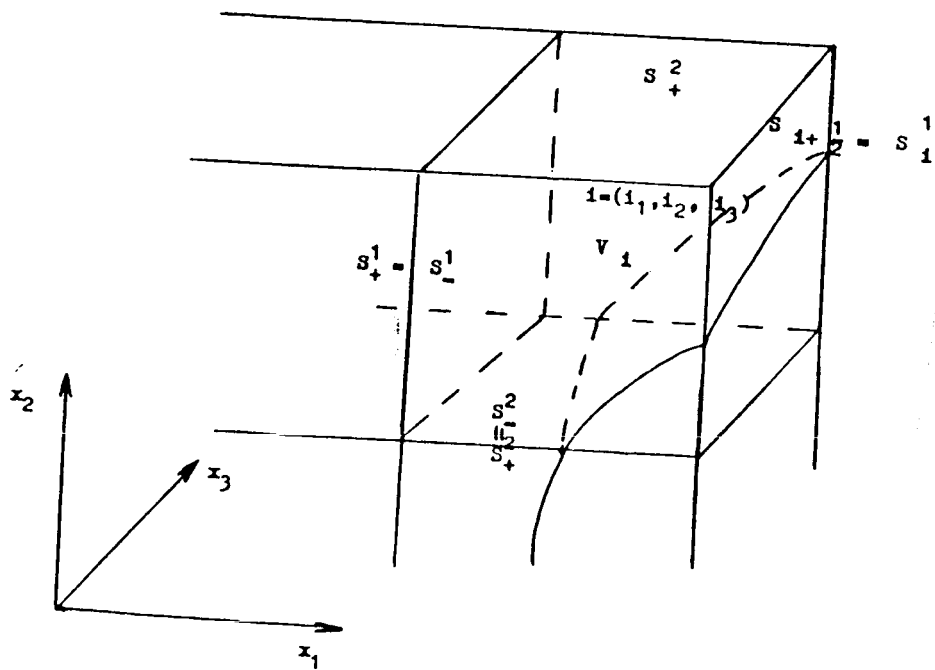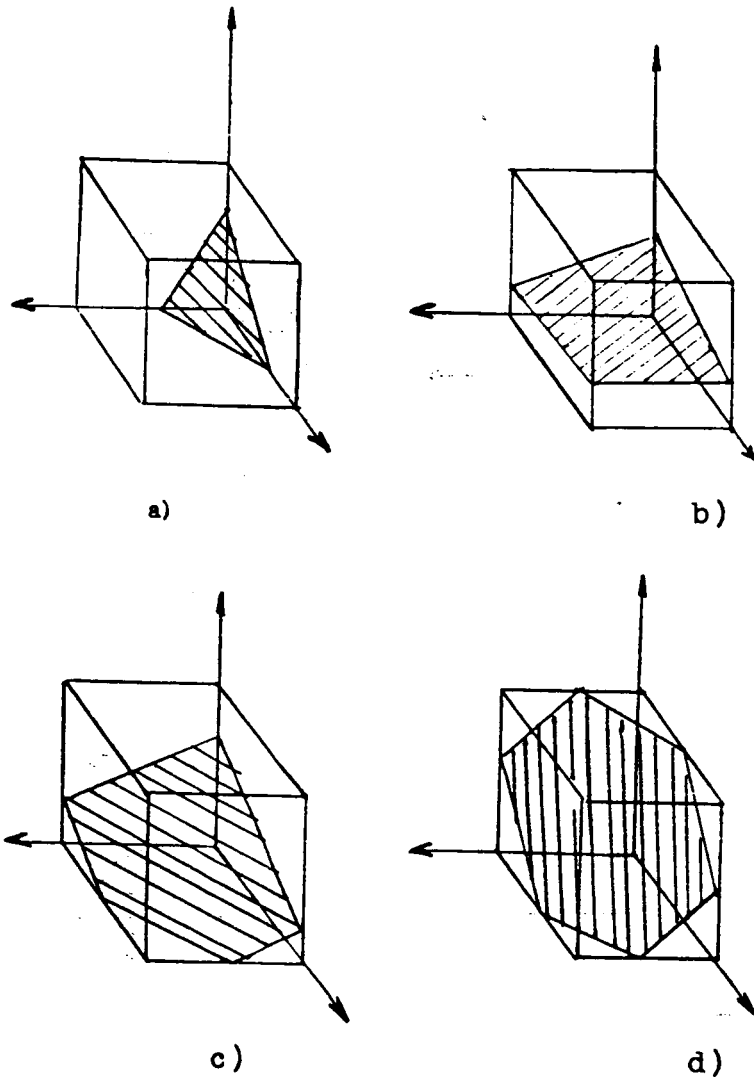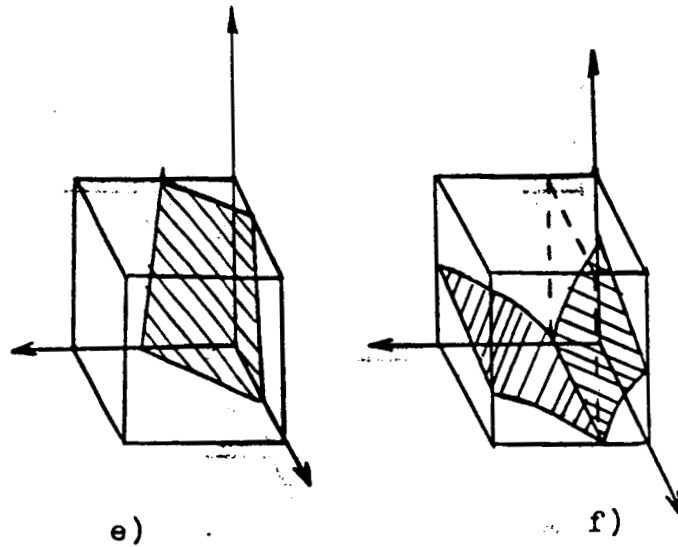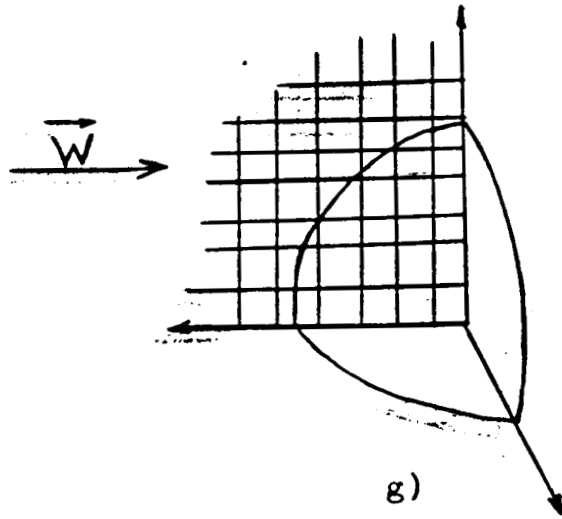
g)

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7

ГРА8ПР CAM FC

Fig. 8a

Fig. 8b

Fig. 8c

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16. Abstract

A method is described for 3D-gasdynamics computer sim-ulation in regions of complicated shape by means of non-adjusted rectangular grids providing unified treatment of various problems. Some test problem computation results are given.

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