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SEVERAL COMPUTER STUDIES ON BOLTZMANN FLOWS IN CONNECTION WITH SPACE FLIGHT PROBLEMS

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Abstract

This report contains the following three papers about computations of rarefied gas flows:

- a) Rarefied gas flow around a disc with different angles of attack, published in the proceedings of the 17th RGD Symposium, Aachen, 1990
- b) Hypersonic flow calculations around a 3D-deltawing at low Knudsen numbers, published in the proceedings of the $17^{\rm th}$ RGD Symposium, Aachen, 1990
- c) Rarefied gas flow around a 3D-deltawing, published in the proceedings of the Workshop on Hypersonic Flows for Reentry Problems, Part 1, Antibes, France, January 22-25, 1990.

All computations are part of the HERMES Research and Development Program.

RAREFIED GAS FLOW AROUND A DISC WITH DIFFERENT ANGLES OF ATTACK

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In this paper we will present a comparison between measurements from a windtunnel and calculations performed by the Finite-Point-set-Method (FPM) for solving the Boltzmann equation. The case considered is the flow around a circular disc at different angles of attack. The comparison covers the whole range of Knudsen numbers from nearly continuum flow (Kn = 0.1) to nearly free molecular flow (Kn = 20.). Furthermore we will investigate the dependence of the aerodynamic coefficients on different gas-surface interaction models, especially the Maxwell-model with an accomodation coefficient. The measurements shown in this paper were performed by Legge, DLR Goettingen, FR Germany.

I. Introduction

Due to the european space project HERMES there is a growing interest in fast and reliable codes for the numerical calculation of flow fields around bodies in the range of free molecular flow, rarefied gas and transition regime. The codes mostly used so far are based on the DSMC method introduced by Sird [1] in 1968. This method is based on the following philosophy [2]: one tries to imitate the microscopic behavior of the gas on the computer and does not care for any clear mathematical formulation of the problem. DSMC is very successful in practice but from a mathematical point of view unsatisfactory since questions about the quality of the approximations can only be answered in test cases and not in terms of general statements independent of a specific situation. As an alternative to this method we developed the Finite-Pointset-Method (FPM), which is directly related to the Boltzmann equation and does not suffer from a lack of mathematical foundation. In chapter II we shortly describe the ideas of the FPM for the case of a monoatomic gas. The more general case of gases with internal degrees of freedom is discussed in [4]. To show the practical efficiency of the method we implemented a code to calculate the 3d-flow field around a flat disc with different angles of attack. In this special case we have the opportunity to compare our numerical results with experimental data obtained by Legge [6] for Knudsen numbers ranging from near continuum regime up to near free molecular flow. In the present paper we show the results for a monoatomic gas. A comparison of the results for a diatomic gas can be found elsewhere [6]. The computational data to perform these calculations are described in

The computational data to perform these calculations are described in chapter III. In chapter IV we describe the calculated aerodynamic coefficients. In the last chapter of the paper we discuss the influence of the specific gas-surface interaction model on the aerodynamic coefficients.

II. The Finite-Pointset-Method

The FPM is a numerical method to solve the Boltzmann equation, which describes in the case of a monoatomic gas the evolution of a positionvelocity space distribution function f(t,x,v) with $x \in \Omega \subset R^3$, $v \in R^3$. The basic idea we use is [3]: approximate a given density function by a finite point set $\omega_N = \{(x_1, v_1), \dots, (x_N, v_N)\}$, such that ω_N converges to f with N tending to infinity.

What we have to define is a distance between ω_{N} and f. This distance will be explained here in a simple one-dimensional situation - the extension to the higher dimensional case can be found in [3]. Let $f:[a,b] \rightarrow R$ be a non-negative function with

$$\int_{[a,b]} f(x) dx = 1$$

an approximation of f by a finite point set (for a sketch see figure 1). We define the discrepancy of ω_{N} with respect to f by

$$D(\omega_{N},f) = \sup_{\left[a',b'\right] c \left[a,b\right]} \left| \int_{\left[a',b'\right]} f(x) dx - \frac{1}{N} \#\left\{x_{i} : x_{i} \varepsilon \left[a',b'\right]\right\} \right|$$

1) We call a sequence of finite points a convergent approximation of f if its discrepancy tends to zero if N tends to infinity.

2) For every fixed N one has to find the sequence ω_N^* , which minimizes the discrepancy with respect to f. ω_N^* is called the optimal approximation of f.

3) The expectation values of functions Φ with respect to f can be approximated by averages of Φ over $\boldsymbol{\omega}_{\boldsymbol{N}}$ with accuracy

$$\left|\int \Phi(x)f(x)dx - \frac{1}{N} \Sigma \Phi(x_i)\right| \leq Var(\Phi)D(\omega_N, f)$$

where $Var(\Phi)$ is the variation of Φ [3].

The general concept of FPM can now be formulated as follows :

(1) Given the initial value f^0 , find a good approximation by a finite pointset $\omega_N^0 = \{(x_1^0, v_1^0), \dots, (x_N^0, v_N^0)\}$.

(2) Find a time evolution of the points

 $t_{j} \rightarrow \omega_{N}(t_{j}) = \{(x_{1}(t_{j}), v_{1}(t_{j})), \dots, (x_{N}(t_{j}), v_{N}(t_{j}))\}$ with $\omega_N(0) = \omega_N^0$ such that $\omega_N(t_j)$ is a good approximation of $f(t_j, \ldots, \ldots)$, the solution of the Boltzmann equation at time $t_j = j \cdot \Delta t$.

One may express this concept also by saying that one has to find an algorithm constructing for each N a ω_N^0 such that $D(\omega_N^0,f^0) \to 0$ and one has to find an evolution $\omega_N(t_j)$ such that $D(\omega_N(t_j),f(t_j)) \to 0$ for 0≦t_i≦T.

III.Calculations performed with the FPM

The FPM algorithms described in [3] and [4] for monoatomic and polyatomic gases respectively can be implemented in such a way that the resulting code is almost completely vectorized.

In all our calculations we used a rectangular grid which was built up by cubes of the same size. In the presented calculations of flows of monoatomic gases the number of points was limited by 200.000. The total number of time steps needed to reach the stationary state and to perform time averaging to smooth the data was 150 in each

We have used the VP100 vector computer of Fujitsu, which has a peak performance of 285 MFLOPS. The mean performance in our calculations was about 60 MFLOPS. The maximum CPU time to perform a single run was 420 seconds, the required main storage was lower than 11 MBytes in each case.

These data show that our code makes it possible to perform extensive parameters studies for the input data:

instream velocity: Ma = 15.6, instream temperature: 2.3 K

Knudsen number: 0.1 - 20, angle of attack: 45° , 60° , 75° , 90° ,

- gas-surface interaction law: Maxwell interaction with variable accomodation coefficient
- wall temperature: 189.8 K, which is the stagnation temperature.

IV. Aerodynamic coefficients

The results we obtained from our calculations may be divided into two parts:

- qualitative values such as density field, temperature field, and Mach field
- quantitative values: the aerodynamic coefficients. Although the qualitative values can be very instructive to visualize the properties of the flow, they are not easy to handle in experimental considerations.

For quantitive values the situation is quite different from the point of view of the experimentalists: they can be measured quite accurately. In addition aerodynamic coefficients are the deciding parameters for the construction of a space shuttle, take for example the lift-to-drag ratio. Therefore the numerical results for these values should agree as well as possible with the measured ones. Figure 2 shows a comparison of calculated and measured values for the drag coefficient, figures 3, 4 and 5 show the comparison for lift, pressure drag and friction drag respectively. As can be seen the main differences arise in the case of the lift coefficient for high Knudsen numbers, the worst case error being about 22%. The mean error in this case is however about 6% which lies in the range of the experimental inaccuracy.

V. Dependence of aerodynamic coefficients on the gas-surface interaction model

As shown in chapter IV. the comparison between measurements and calculation with complete accomodation as gas-surface interaction is not content in each cases. Especially for the lift coefficient at high Knudsen numbers we get unsatisfactory results. However the numerical results tend to the analytical value of the free molecular limit. The reason for this difference can be found by considering the models used for the mathematical description of the gas by the Boltzmann-Equation. One necessary model for the dynamic description is the collision model, for example the hard-sphere gas in the actual calculation. The other modelisation of nature is done by a simple description of the gas-surface interaction. The aerodynamic coefficients now seem to be more sensitive to the gas-surface interaction model than to the collision model.

Therefore we will give an investigation about the influence of an accomodation coefficient to the integrated surface properties. We will focus especially on the Maxwell-model, which is given as a linear combination of complete accomodation and specular reflection. In the free molecular limit one can calculate analytically, that the aerodynamic coefficients are given as the same linear combination of the value for complete accomodation and specular reflection. For small Knudsen numbers one will espect just a small change in the coefficients. In the transitional regime it is possible to cover the dependence on the accomodation coefficient by a simulation method. We will present simulation results for two different Knudsen numbers, namely 0.1 and 5.0, at an angle of attack of 45 degrees. Calculations were performed for accomodation coefficients ranging from 0.0 (specular reflection) to 1.0 (complete accomodation) with a stepsize

of 0.1.

Figure (6) shows the drag coefficient, figure (7) the the lift coefficient, figure (8) the pressure-drag coefficient and finally figure (9) the friction-drag coefficient.

For the large Knudsen number 5.0 we get the expected linear behavior of the aerodynamic coefficients. For the small Knudsen number the influence of the accomodation coefficient is much weaker and we get a nonlinear dependence on the accomodation coefficient.

VI. References

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Computational Methods for the Boltzmann-Equation, AGTM report
No 43, University of Kaiserslautern 1990

[4] S.Koerber, B.Wiesen:
A Comparison of a Microscopic and a Phenomenological Model for a Polyatomic Gas, to appear in AGTM reports, University of Kaiserslautern

[5] H.Legge: Force and Heat Transfer Measurements on a Disc at 45°-90° Angle of Attack in a Free Jet Flow Using Ar, He, N₂, H₂ as Test Gases, DLR IB 222 - 89 A 07 (1989)

[6] J.Struckmeier, B.Wiesen:
Flow of a Rarefied Diatomic Gas around a Disc with Different
Angles of Attack, to appear

f(v)

Fig. 1 : Schematic approximation of a function by a finite pointset

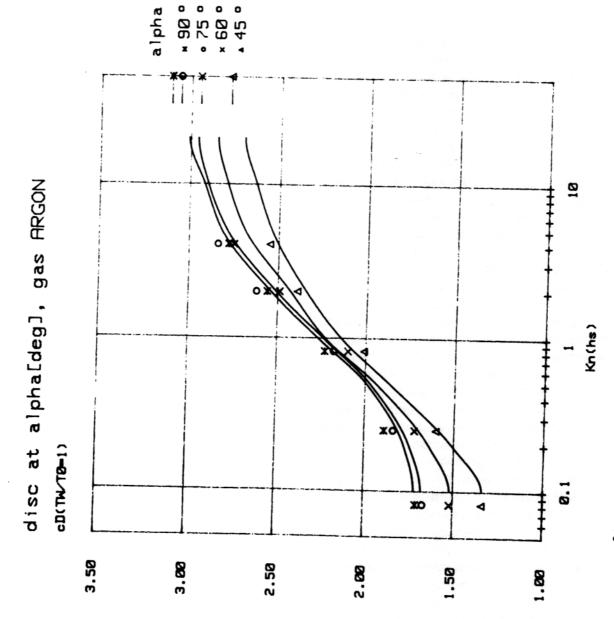
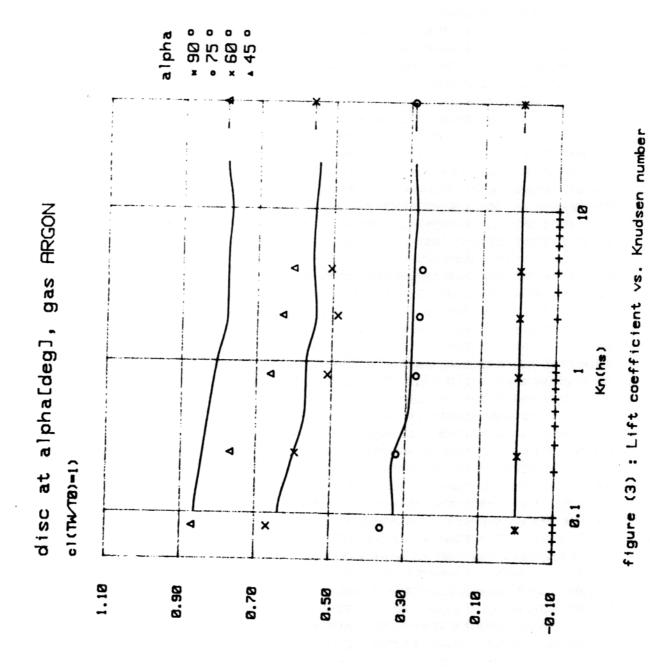


figure (2) : Drag coefficient vs. Knudsen number



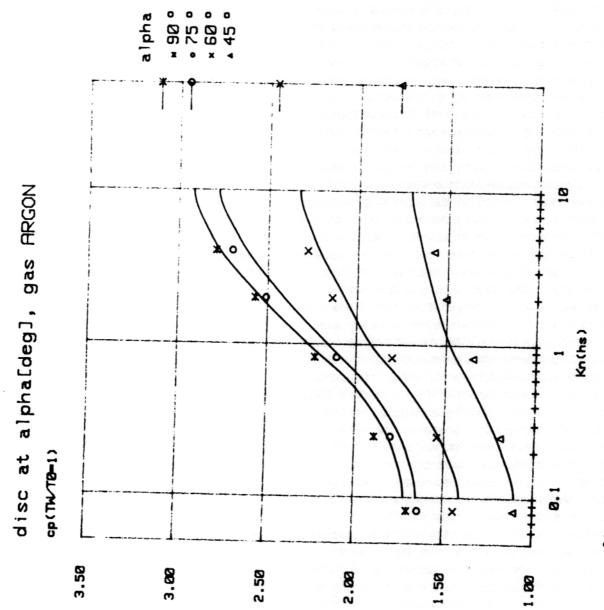


figure (4) : Pressure drag coefficient vs. Knudsen number

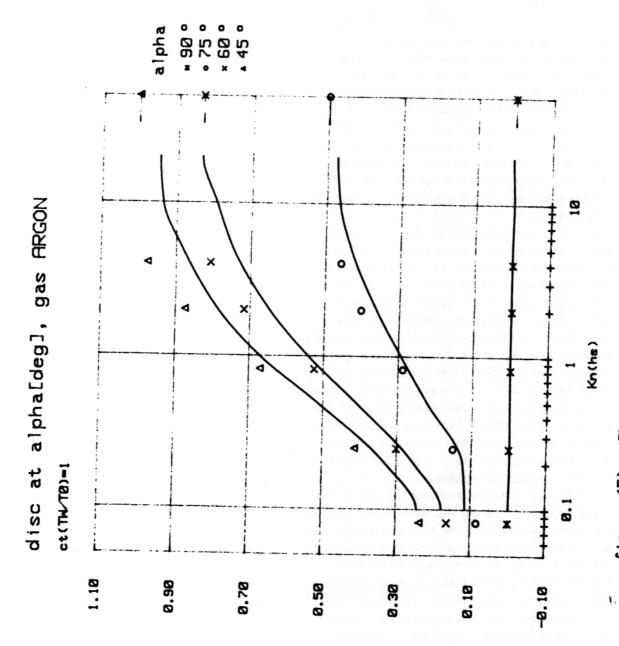
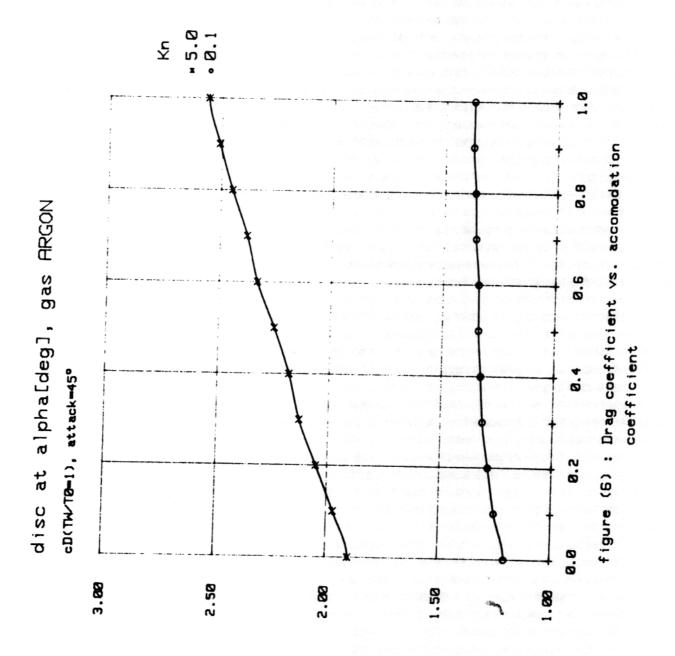
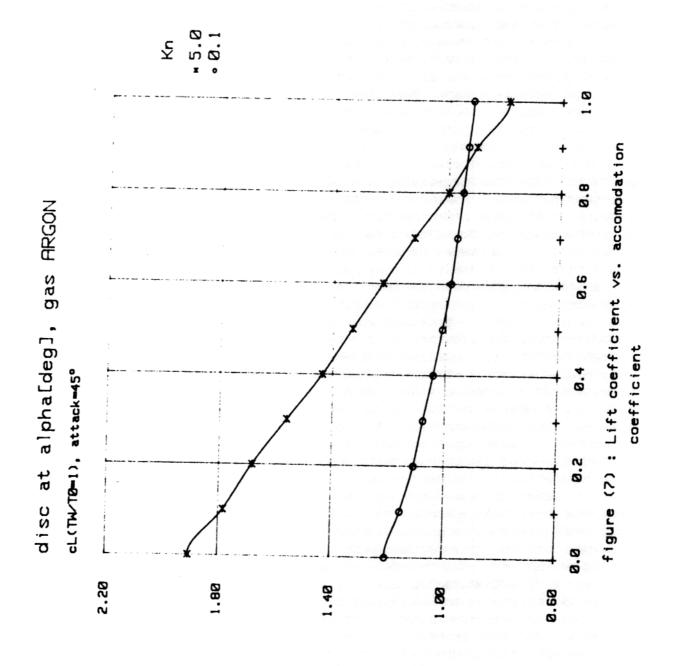
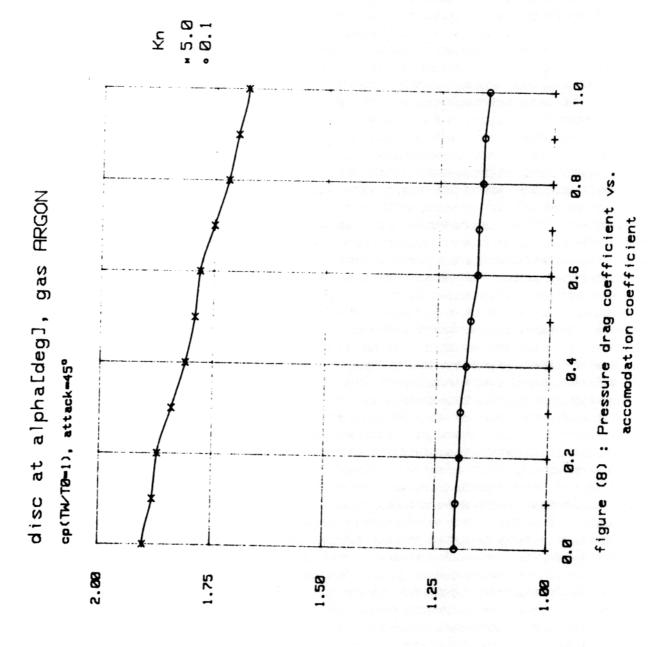
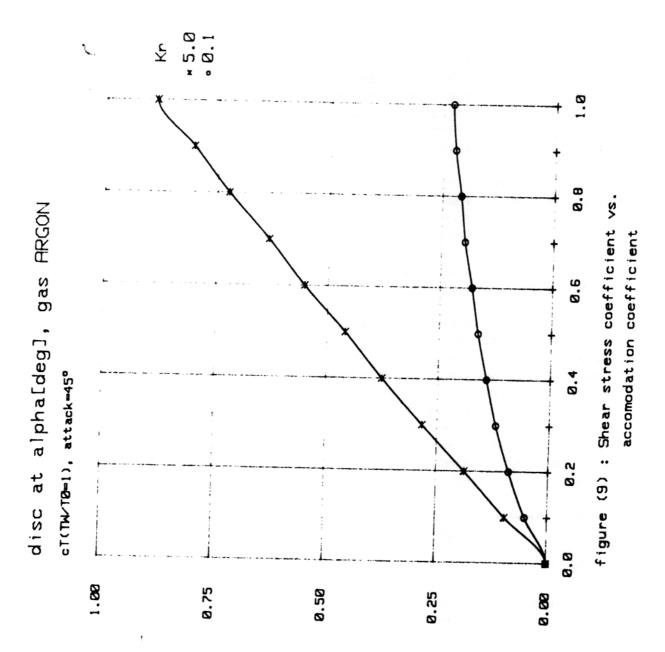


figure (5) : Shear stress coefficient vs. Knudsen number









HYPERSONIC FLOW CALCULATIONS AROUND A 3D-DELTAWING AT LOW KNUDSEN NUMBERS

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This paper presents numerical results for hypersonic flows around a 3d-deltawing at low Knudsen numbers, i.e. near the continuum regime. The underlying body geometry corresponds to one of the testcases on rarefied gas regime proposed for the workshop on hypersonic flow, which was held in Antibes, France, January 1990. The numerical method used in the calculations is the so-called Finite-Pointset-Method (FPM) developed at the university of Kaiserslautern during the last year. The paper shows that the FPM is an efficient alternative method beside the well-known Monte-Carlo-methods (DSMC).

I. Introduction

In this paper we will focuse only on the numerical results and the computational effort of the FPM. The theoretical part of the FPM and a detailled description of the method can be found in reference [1]. The flow around a 3d-body at low Knudsen numbers is a pretentious testcase for numerical methods in the rarefied gas regime.

The geometry of the deltawing is shown in figure 1. The Knudsen number in this case is defined by the ratio between the mean free path and the length of the deltawing.

II. Numerical results

We will present calculations at a Knudsen number of 0.01 and 0.1 in the case of the monatomic gas Argon. The case of diatomic gas Nitrogen with a Larsen-Borgnakke model can be found in reference [2]. The angle of attack was 30 degree in both cases. The wall temperature was fixed at 620 K, the instream temperature 13.5 K and the Mach Number 20.2. The gas-surface-interaction was complete accommodation and the particle collision were performed by a hard-sphere-scattering. The following table gives the results for integrated surface quantities at a Knudsen number 0.01:

heat transfer coefficient	C _H =0.38
pressure-drag coefficient	C _{DP} = 1.29
friction-drag coefficient	$C_{DF} = 0.04$
lift coefficient	C _L = 0.74
drag coefficient	C _D = 1.05

The following figures present results for a Knudsen number of 0.1. Figure 2 shows the density contours near the symmetry plane, figure 3 the temperature, figure 4 the Mach contours near the symmetry plane.

Figure 6 to 8 show the corresponding contours in the cross-sectional plane at x/L = .8, where the plane is perpendicular to the upper surface of the deltawing as shown in figure 5.

III. Computational effort

The computational effort of a simulation method in a realistic flow situation depends mainly on three conditions :

- (i) the Knudsen number
 The space discretization of the flowfield, which is necessary to
 perform the collision procedure and the sampling of macroscopic
 quantities, has to be correlated to the Knudsen number. As a consequence the number of cells needed to get a reasonable resolution of
 the flow field increases with a decreasing Knudsen number and the
 ratio between the number of cells and the Knudsen number decreases
 dramatically in three space dimensions.
- (ii) the convergence to the stationary state
 All existing simulation methods try to reproduce the instationary
 flow problem. On the other hand one is mainly interested on the flow
 structure in the stationary state. Therefore the number of timesteps,
 which have to be performed to reach the stationary state, characterize
 the efficiency of a numerical method.
- (iii) the fluctuations in the stationary
 A simulation method produces scattered data, because of the finite number of points, which approximate the exact gas distribution. To get smooth data it is necessary to perform time averaging procedures in the stationary state. Dependent on the quality of a single simulation step, the number of timesteps, which are necessary to reach the stationary state.

The required CPU-time at a Knudsen number of 0.01 was 7.5 hours. The calculations were performed at a Siemens VP100 at the university of Kaiserslautern with a peak performance of 285 MFLOPS (3.5 hours) and at a Siemens VP400 at the university of Karlsruhe with a peak performance of about 1.140 MFLOPS (4 hours). The required main storage was 63 MB at the VP100 and 183 MB at the VP400. The number of particles used in the simulation was about 3.6 millions and the number of cells increases from about 15.000 at the beginning to about 70.000 in the stationary state. 6.5 hours were needed to reach the stationary state, mainly to build up the adaptive grid structure and 1 hour was needed to perform the time averaging procedure. At larger Knudsen numbers and more rarefied flow conditions the CPU-time is much less than above, for example about 1 hour at Kn = 0.1. In the case of diatomic gas (including the Larsen-Borgnakke model for the internal energy) the required CPU-time was about 20% higher.

IV. References

[1] F.Gropengiesser, H.Neunzert, J.Struckmeier:
Computational methods for the Boltzmann equation, Berichte der
Arbeitsgruppe Technomathematik, Universitaet Kaiserslautern, to
appear in "Venice 1998: The State of Art in Appl. and Industrial
Math.", ed. R. Spigler, Kluwer acad. publ., 1990.

[2] F.Gropengiesser, H.Neunzert, J.Struckmeier, B.Wiesen: Hypersonic flow calculation around a deltawing, Workshop on Hypersonic flows, Antibes, France, 1990, in preparation.

Fig. 1 : Geometry of the deltawing

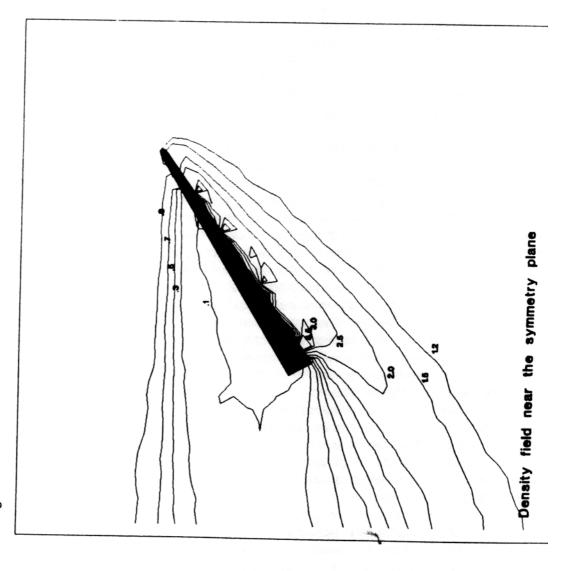


Fig. 2

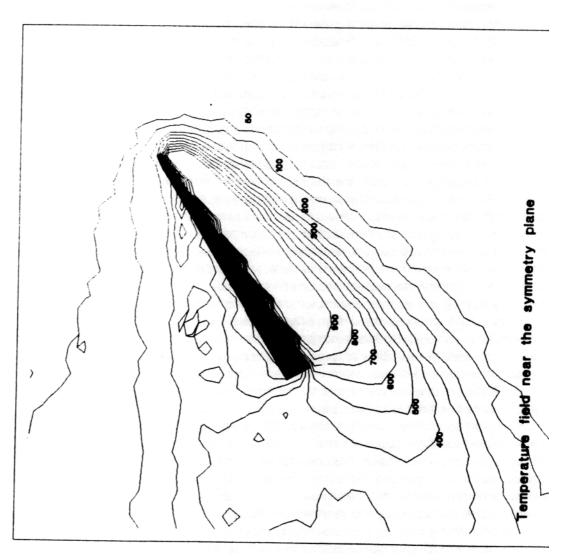


Fig. 3

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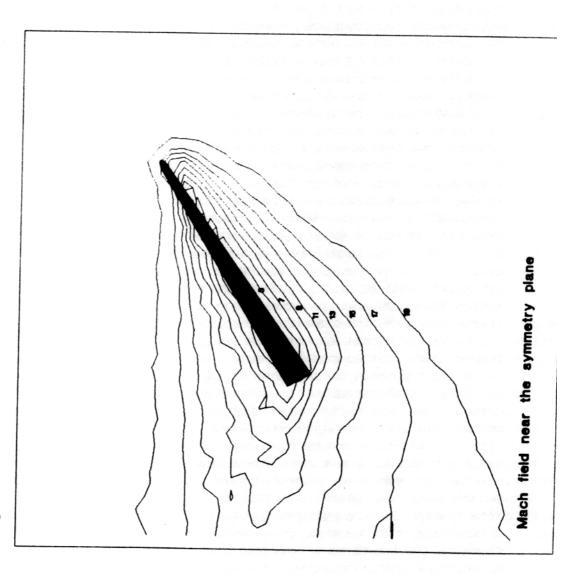
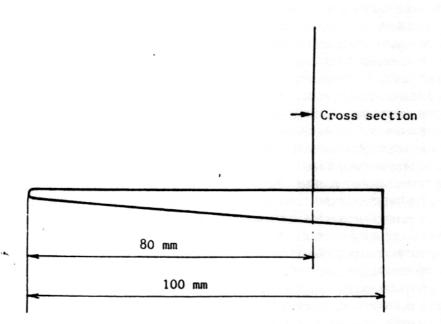
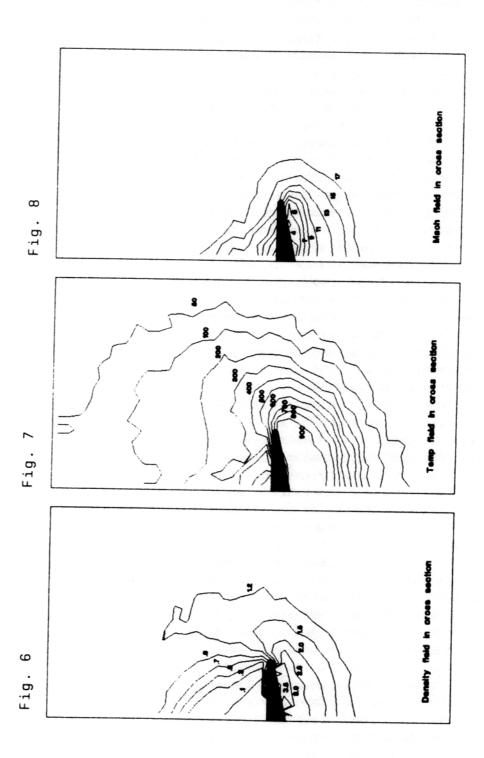


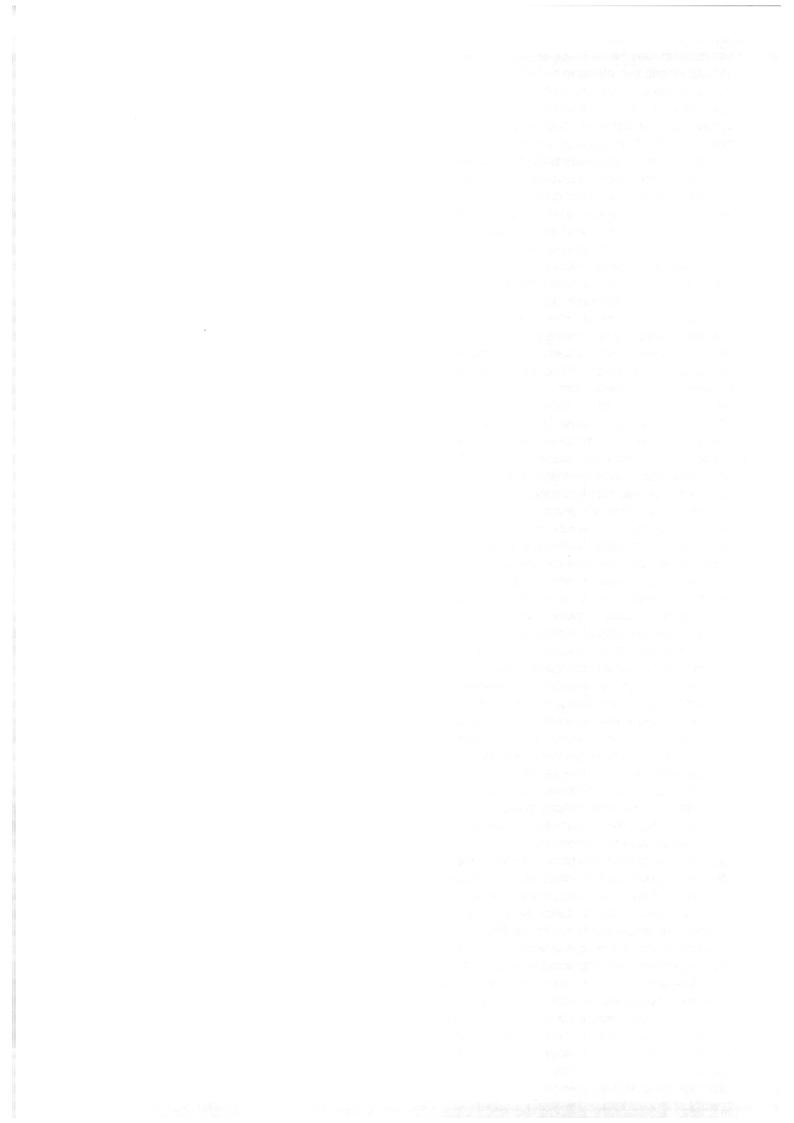
Fig. 4

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Fig. 5 : Cross sectional plane at x/L = 0.8







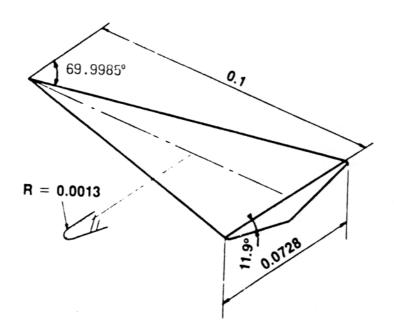
Rarefied Gas Flow Around A 3D-Deltawing

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This paper presents numerical results for hypersonic flows around a 3D-deltawing at a low Knudsen number. The underlying body geometry as well as the physical parameters correspond to testcase 7.2.1. of the workshop. The numerical method used for the calculations is the Finite-Pointset-Method (FPM) developed at the University of Kaisers-lautern since 1987. The paper gives a short introduction to the method and then follows the required output formats of the workshop. Further calculations can be found in [3],[4].

Figure 1: Illustration of the deltawing



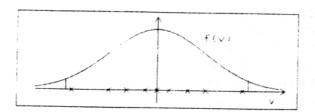
1 The Finite Pointset-Method

The FPM is a numerical method to solve the Boltzmann equation, which describes in the case of a monoatomic gas the evolution of a position-velocity space distribution function f(t,x,v) with $x \in \Omega \subset R^3$, $v \in R^3$. The basic idea we use is [1]: approximate a given density function by a finite point set $\omega_N = \{(x_1,v_1), \dots, (x_N,v_N)\}$, such that ω_N converges to f with N tending to infinity.

What we have to define is a distance between ω_N and f. This distance will be explained here in a simple one-dimensional situation - the extension to the higher dimensional case can be found in [1]. Let $f:[a,b] \to R$ be a non-negative function with

$$\int_{[a,b]} f(x)dx = 1$$

and ω_N an approximation of f by a finite point set (for a sketch see the following figure).



We define the discrepancy of ω_N with respect to f by

$$D(\omega_N, f) = \sup_{[a', b'] c[a, b]} | \int_{[a', b']} f(x) dx - \frac{1}{N} \# \{ x_i : x_i \in [a', b'] \} |$$

- 1. We call a sequence of finite points a convergent approximation of f if its dicrepancy tends to zero if N tends to infinity.
- 2. For every fixed N one has to find the sequence $\omega_N *$, which minimizes the discrepancy with respect to f. $\omega_N *$ is called the optimal approximation of f.
- 3. The expectation values of functions Φ with respect to f can be approximated by averages of Φ over $\omega_N *$ with accuracy

$$|\int \Phi(x)f(x)dx - \frac{1}{N}\sum \Phi(x_i)| \le Var(\Phi)D(\omega_N, f)$$

where $Var(\Phi)$ is the variation of Φ [1].

The general concept of FPM can now be formulated as follows:

- 1. Given the initial value f^0 , find a good approximation by a finite pointset $\omega_N^0 = \{(x_1^0, v_1^0), \dots, (x_N^0, v_N^0)\}.$
- 2. Find a time evolution of the points

$$t_j \to \omega_N(t_j) = \{(x_1(t_j), v_1(t_j)), \cdots, (x_N(t_j), v_N(t_j))\}$$

with $\omega_N(0) = \omega_N^0$ such that $\omega_N(t_j)$ is a good approximation of $f(t_j, \dots, \dots)$, the solution of the Boltzmann equation at time $t_j = j \cdot \Delta t$.

One may express this concept also by saying that one has to find a algorithm constructing for each N a ω_N^0 such that $D(\omega_N^0, f^0) \to 0$ and one has to find a evolution $\omega_N(t_j)$ such that $D(\omega_N(t_j), f(t_j)) \to 0$ for $0 \le t_j \le T$.

2 Results of calculations for testcase 7.2.1.: (testgas Nitrogen N_2)

I. General data

a) computer : i. VP 400 Fujitsu

: ii. VP 100 Fujitsu

main storage : i. 256 Mbyte main storage unit

256 Mbyte vector storage unit

ii. 128 Mbyte main storage unit

maximal performance : i. 1140 Mflops

ii. 285 Mflops

mean performance : i. 90 Mflops

ii. 60 Mflops

b) required cpu-time : 12.5 hours

(7.5 h on the VP400, 5h on the VP 100)

required computer storage : 199 Mbyte on the VP 400

76 Mbyte on the VP 100

c) cpu-time until stationary state : 11 hours

(6h on the VP 400, 5 h on the VP 100)

cpu-time for averaging : 1.5 hours on the VP 400 d) collision model : Larsen-Borgnakke model gas-surface-interaction model : complete accommodation

e) The mean free path of the upstreaming gas is defined in the usual way [2]

$$\lambda_{\infty} = \frac{c'}{n \frac{c}{\sigma_T c_r}}$$

(c' mean spead, c_r relative velocity, σ_T total cross section n number density). The Knudsen number is given by

$$K_n = \frac{\lambda_{\infty}}{L}$$

(L chord length)

Transport coefficients can be calculated by using Ω -integrals. Because of the high Mach number of the upstreaming gas we used the hard sphere total cross section, where the only free parameter is the sphere diameter. The value for this parameter was given by the N_2 diameter.

- f) $n_{\infty} = 4,65 \cdot 10^{20}/m^3$
- g) upstream boundary condition: Maxwellian with $\rho_{\infty}, u_{\infty}, T_{\infty}$

II. Gridstructure

a) An adaptive grid consisting of cubes is used. Starting with coarse cells the grid is refined during the first timesteps and then every tenth timestep. After about 60 timesteps the grid stagnates.

initial number of cells: 15750 final number of cells: 71040

b) Figure 2: 3-D illustration of the final grid

III. Flowfield results for plane of symmetry:

Figure 3: Density contours near the symmetry plane

Figure 4: Mach number contours near the symmetry plane

Figure 5: Translational temperature contours near the symmetry plane

Figure 6: Internal temperature contours near the symmetry plane

IV. Flowfield results for a cross flow plane

Figure 7: Density contours in the cross flow plane

Figure 8: Mach number contours in the cross flow plane

Figure 9: Translational temperature contours in the cross flow plane
Figure 10: Internal temperature contours in the cross flow plane

V. Stagnation streamline results

Figure 11: Density along the stagnation streamline

Figure 12: Translational temperature along the stagnation streamline Figure 13: Internal temperature along the stagnation streamline

VI. Overall forces

1. heat-transfer coefficient $C_H = 0.276$

2. pressure-drag coefficient $C_{DP} = 1.32$

3. friction-drag coefficient $C_{DF} = 0.039$

4. lift coefficient $C_L = 0.72$

5. drag coefficient $C_D = 1.06$

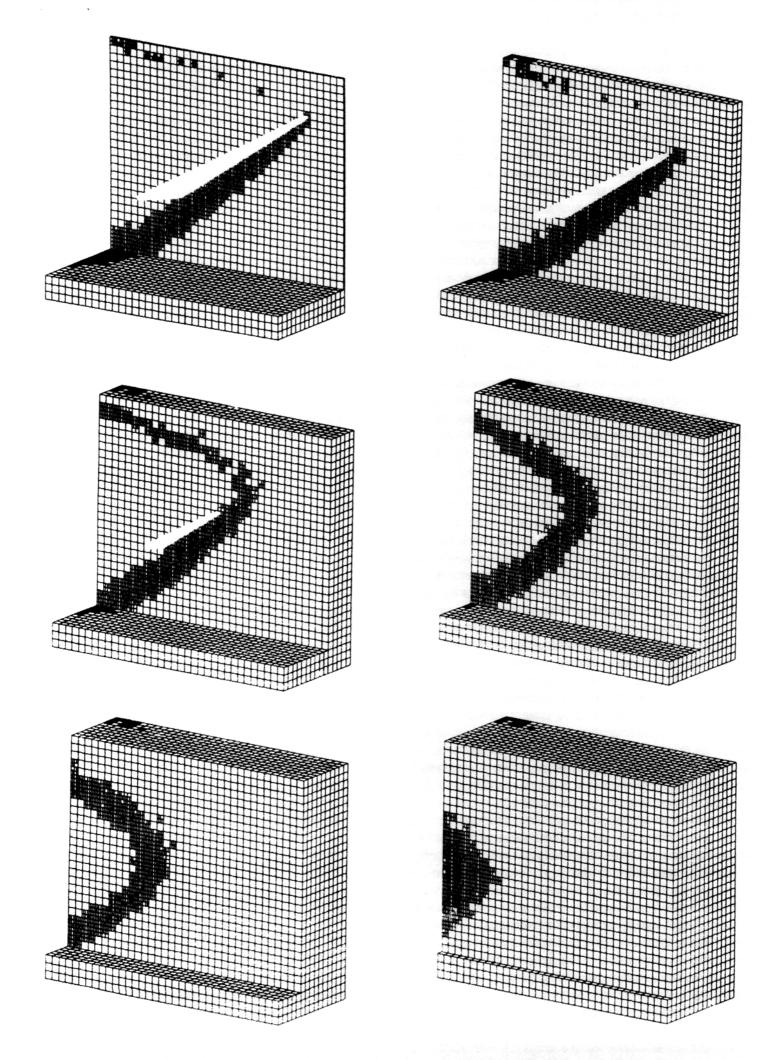
 C_{DP} and C_{DF} are normalized by the projection of the surface area and not by the surface area itself.

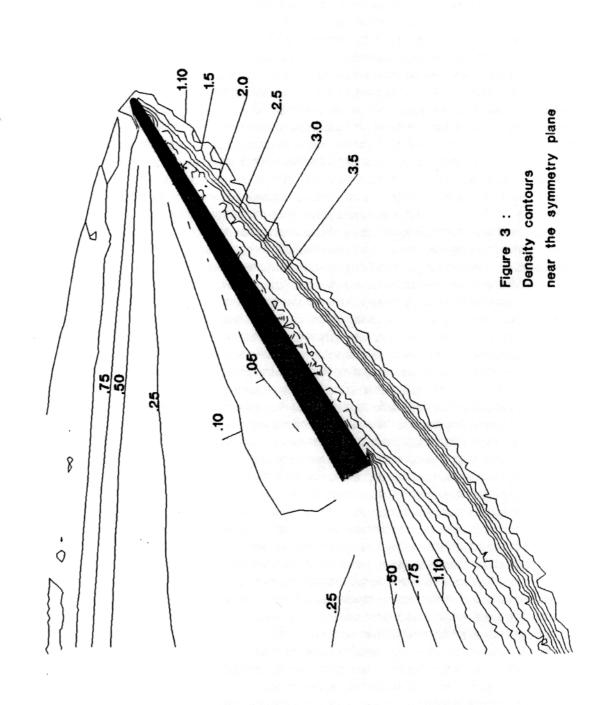
VII. Convergence History

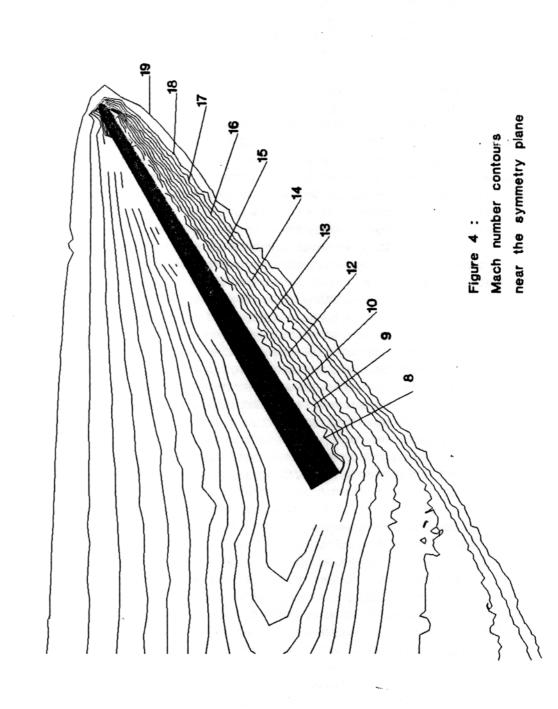
Figure 14: drag coefficient versus simulation time

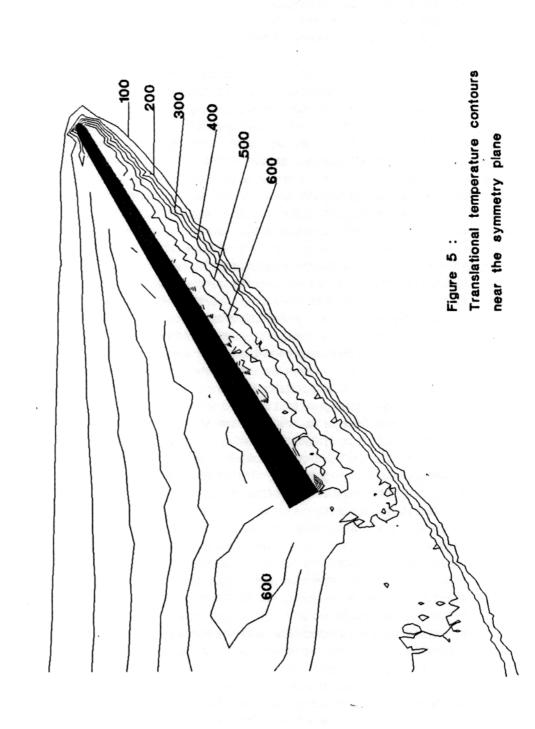
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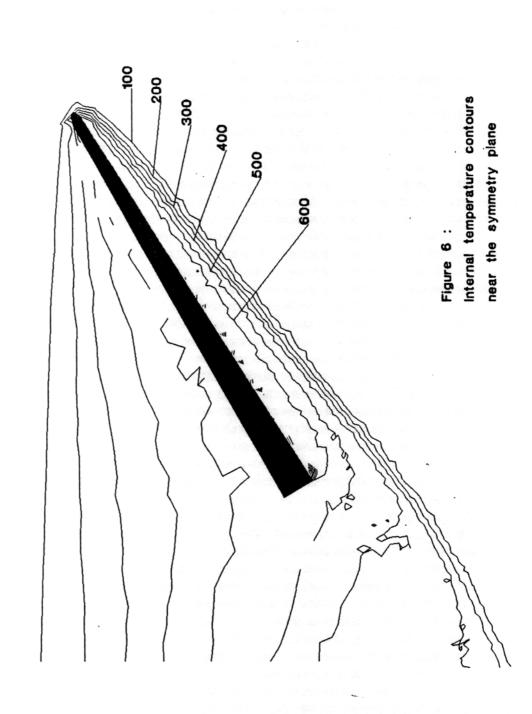
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- [3] F. Gropengießer, H. Neunzert, J. Struckmeier, B. Wiesen: Rarefied Flow around a Disc with different angles of attack, to appear in the proc. of the 17th RGD-Symposium, Aachen 1990
- [4] F. Gropengießer, H. Neunzert, J. Struckmeier, B. Wiesen: Hypersonic Flow Calculations around a 3D-Deltawing at low Knudsen numbers, to appear in the proc. of the 17th RGD-Symposium, Aachen 1990











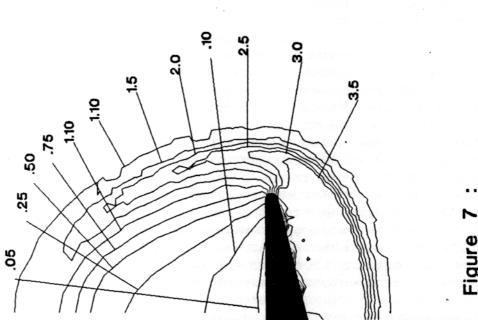


Figure 7 :
Density contours
at cross section x/L = 0.8

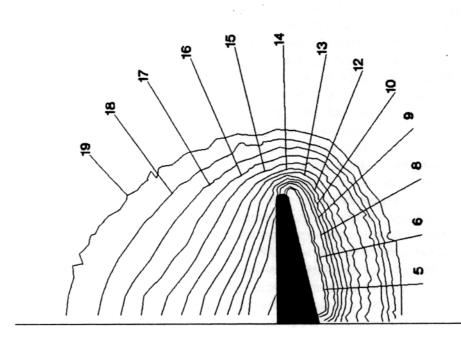


Figure 8 :
Mach number contours
at cross section x/L = 0.8

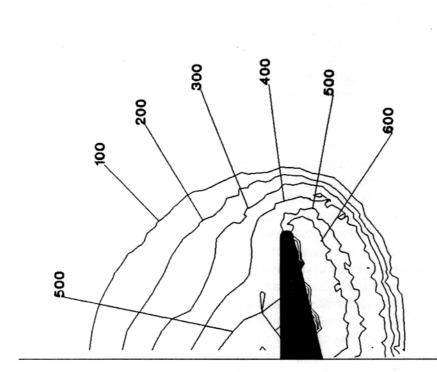


Figure 9 : Translational temperature contours at cross section x/L=0.8

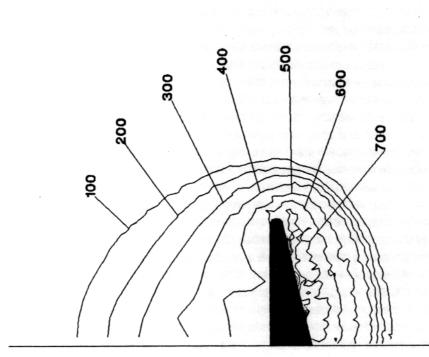


Figure 10 : Internal temperature contours at cross section x/L = 0.8

