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An Open Source, Parallel DSMC Code for Rarefied Gas Flows in Arbitrary Geometries

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Abstract

This paper presents the results of validation of an open source Direct Simulation Monte Carlo (DSMC) code for general application to rarefied gas flows. The new DSMC code, called *dsmcFoam*, has been written within the framework of the open source C++ CFD toolbox OpenFOAM. The main features of *dsmcFoam* code include the capability to perform both steady and transient solutions, to model arbitrary 2D/3D geometries, and unlimited parallel processing. Test cases have been selected to cover a wide range of benchmark examples from 1D to 3D. These include relaxation to equilibrium, 2D flow over a flat plate and a cylinder, and 3D supersonic flows over complex geometries. In all cases, *dsmcFoam* shows very good agreement with data provided by both analytical solutions and other contemporary DSMC codes.

Keywords: DSMC, open-source, object-oriented, rarefied gas, benchmark, complex geometry, parallel.

1. Introduction

The Direct Simulation Monte Carlo (DSMC) method [1,2] is the dominant numerical technique for solving engineering problems where the flow is rarefied. When applied properly, solutions to very complex flows involving chemical reactions, ionization and high degrees of molecular non-equilibrium are achievable. Examples of such flows range from planetary spacecraft re-entry [3-5] to micro and nano scale gas flows [6-8]. Reviews of work in the field of DSMC can be found in the literature [9-11].

The dimensionless parameter describing the degree of gas rarefaction is the Knudsen number

$$Kn = \frac{\lambda}{L} \tag{1}$$

i.e., the ratio of the mean free path of the gas molecules, λ, to the characteristic dimension of the flow, L. When the gas is sufficiently rarefied (Kn ~ 0.01), solutions obtained using conventional Navier-Stokes

CFD methods [4-6] are inadequate, while practical solutions to the fundamental governing Boltzmann equation have proven to be complicated and time-consuming.

The basis of the DSMC method, first formulated by Bird in the 1970's [2], is to circumvent the direct solution of the Boltzmann equation by considering a probabilistic simulation. It is categorized as a particle method, in which each simulation particle represents a large number of real gas atoms or molecules. The physics of the gas is captured by uncoupling the motion of the particles from their collisions. In a similar manner to conventional CFD, the implementation of DSMC normally requires the decomposition of the computational domain into a collection of grid cells. After molecular movements have taken place, the collisions between particles are simulated in each cell in a probabilistic manner and a statistical picture of the flow phenomena is built up. With the advent of high performance parallel computing (HPC) architectures, ensembles of DSMC simulator particles in large 3D problems can be of the order of 10^8 (however practical solutions to engineering problems in smaller 2D geometries may be achieved nowadays within realistic time scales using a modest PC [12]).

The DSMC code presented in this paper has been formally titled *dsmcFoam* and is based on Bird's original formulation [2]. The open source nature of the new code, its unlimited parallel solution capability, and its potential application to 3D, arbitrary geometries are highlighted. All of these may be considered as distinguishing features when compared with currently available DSMC codes.

2. Code Development

dsmcFoam has been developed within the framework of the open source CFD toolbox OpenFOAM [13]. The code has been written, with collaboration from the authors, by OpenCFD Ltd., for release in OpenFOAM version 1.6. OpenFOAM is a flexible set of efficient, object-oriented C++ modules for solving complex fluid flows. It is freely available and open source under the GNU general public licence. A pre-existing molecular dynamics (MD) code contained within OpenFOAM [14-16] has been modified to generate the new DSMC capability (*dsmcFoam*). Fundamental features of the existing MD code including particle initialisation in arbitrary geometries and particle tracking in unstructured, arbitrary, polyhedral meshes are among the core elements of the new *dsmcFoam* code.

The OpenFOAM CFD toolbox has been developed in C++; the flexible, modular nature of the C++ coding blocks and the source code access mean that user-modified coding for new DSMC models is relatively easy to implement. Furthermore, the hierarchical structure of the code and the inheritance features of the coding blocks mean that new user-coding (*derived classes*) can inherit essential features (*base classes*) without the need to re-code.

The open source philosophy behind OpenFOAM means that commercial CFD licensing costs are eliminated while the unlimited parallel processing capability means that practical engineering problems may be tackled within realistic time scales and on modest hardware budgets. The operating system used for the work contained in this paper was the freely available OpenSUSE Linux v11.1.

The current features of *dsmcFoam* may be summarised as follows:

- Steady and transient simulations
- Unlimited parallel processing capability
- Arbitrary 2D/3D geometries
- Automatic sub-cell generation to promote nearest neighbour collisions [1]
- Arbitrary number of gas species
- Freestream flow boundaries [1]
- Variable Hard Sphere (VHS) collision model [1]
- Larsen-Borgnakke internal energy redistribution model [1]
- Diffuse or specular wall reflection boundaries
- Cyclic (periodic) boundaries

The *dsmcFoam* directory structure is shown in Figure 1. The directory tree shows the location of the submodels containing the source code related to the binary collision, inflow boundary and wall-interaction models. The location of the utilities *dsmcFieldsCalc* and *dsmcInitialise* are highlighted in yellow, as is the solver *dsmcFoam*. These utilities and solver are discussed in the following section.

3. General Solution Procedure

In a similar manner to conventional CFD, a numerical mesh is created to describe the physical extent of the flow domain and any solid obstacles within it. Good DSMC practice suggests that the typical cell size should be a fraction of the mean free path, while the time step size should be a fraction of the mean collision time of the gas molecules. Boundary types are then specified to describe the nature of the boundaries (e.g. freestream, specular/diffuse, cyclic etc.) and gas properties are prescribed at these boundaries (e.g. velocity, temperature, number density etc.). All of the meshes (both structured and unstructured) within this paper have been created using OpenFOAM, but translators do exist within OpenFOAM allowing the user to import meshes generated by a range of third-party grid-generation software.

Following the mesh generation and boundary condition prescription three *dsmcFoam* features are run:

1. *dsmcInitialise* – a pre-processing utility to create initial configurations of DSMC particles in arbitrary geometries.
2. *dsmcFoam* – the DSMC solver.
3. *dsmcFieldsCalc* – a post-processing utility to calculate the intensive fields (density, velocity and temperature) from extensive fields (mass, momentum and energy).

The locations of the above utilities and solvers are shown in Figure 1; all can be run in parallel. Furthermore, *dsmcFieldsCalc* can be executed at the runtime of the solver allowing the user to visualise the flow field during a solution. All post-processing is carried out using the open source visualiser Paraview, which is supplied with the OpenFOAM suite.

4. Benchmark testing of *dsmcFoam*

Six benchmark test cases are considered. In all of the cases, the Knudsen number is defined as in equation 1, with the value of the mean free path, λ, determined for either hard sphere (HS) molecules [17] using:

$$\lambda = \frac{16\mu}{5\rho}\left(\frac{m}{2\pi kT}\right)^{1/2} \tag{1}$$

or variable hard sphere (VHS) molecules [17] according to:

$$\lambda = \frac{2(5-2\omega)(7-2\omega)}{15}\left(\frac{m}{2\pi kT}\right)^{1/2}\left(\frac{\mu}{\rho}\right) \tag{2}$$

Where ω is the temperature coefficient of viscosity, m is the atomic mass, k is the Boltzmann constant, T is the temperature, μ is the gas dynamic viscosity and ρ is the gas density. The values of the reference temperature, $T_{ref,}$ and the parameters ω and m are provided in table 1. Also contained in the table are the length scale, L, for the Knudsen number calculation, the type of molecule (HS or VHS) for the definition of λ and the species reference molecular diameter, d_{ref}.

Good DSMC practice [1] suggests that the time-step should be a fraction of the mean free time (the mean time between collisions) at the free stream conditions. This fraction, ξ, is defined as:

$$\xi = \frac{\bar{c}\Delta t}{\lambda} \tag{3}$$

Where $\bar{c} = \sqrt{8kT/\pi m}$ is the mean thermal speed and Δt is the chosen time step. Values of ξ are shown in table 1.

CASE	*Species*	λ *definition*	T_{ref} (K)	ω	d_{ref} ($\times 10^{10}$) (m)	m ($\times 10^{27}$) (kg)	ξ	L (m)
A	*Ar*	HS	273	0.81	4.17	66.3	0.06	1×10^{-6}
B	N_2	VHS	273	0.74	4.17	46.5	0.13	1
C	N_2	VHS	290	0.70	4.11	46.5	0.1	0.02
D	*Ar*	HS	273	0.81	4.17	66.3	0.002	0.305
E	N_2	VHS	273	0.74	4.17	46.5	0.044	0.25
F	*Ar*	VHS	273	0.81	4.17	66.3	0.045	0.02

Table 1 *Molecular parameters for each benchmark case*.

4.1 Benchmark Case A : 1D Relaxation to Equilibrium

This case describes the relaxation to equilibrium of a monatomic Argon gas [18]. The gas exists in a volume of side length 1×10^{-6} m with a density of 1.78 kg/m^3 and temperature of 273 K. Cyclic boundaries are specified everywhere on the domain envelope and the initial particle conditions for the *x*-velocity component is set as a +/- random coin-flip of the most probable thermal speed. The impulsive initial conditions are shown in Figure 2 as a vertical green line. The VHS collision model was employed.

The Knudsen number is 0.064 and 40 cells are created in the *x*-direction with 1 cell in the *y* and *z* directions. Each cell contained an initial 40 DSMC particles to produce a total number of 1600 simulators. The time step size was 1×10^{-11} s. Time averaging was activated at $t = 5 \times 10^{-7}$ s and continued until 1×10^{-6} s producing 83 million samples.

The results are shown in Figure 2 and it is evident that relaxation to the equilibrium Maxwell-Boltzmann distribution has occurred, i.e.

$$P_v(v)\,dv = 4\pi(\frac{m}{2\pi kT})^{3/2} v^2 e^{-0.5mv^2/kT} dv \qquad (3)$$

where $P_v(v)$ is the probability, v is the thermal speed, m is the mass, k is the Boltzmann constant and T the temperature. The particle speed distribution is normalized by assuming that $\int_0^\infty P(v)\,dv = 1$. There is some minor statistical scatter of the *dsmcFoam* results (blue crosses) around the velocity maximum but otherwise the predicted velocities match exactly the analytical velocity distribution shown in red.

4.2 Benchmark Case B : 2D Supersonic Flow over a Flat Plate

This case is the 2D supersonic flow of nitrogen over a flat plate, considered by Bird [1]. The Mach number is 4, the Knudsen number 0.0143, the freestream gas is at a temperature of 273 K, the number density is 1×10^{20} molecules/m^3 and the plate surface temperature is 500 K. Freestream conditions exist at the inlet, outlet and upper boundaries while a short length upstream of the upstream edge of the plate was considered as symmetric. The plate itself was considered to be a diffusive surface and, finally, cyclic conditions were set on all other boundaries. The VHS model was employed for particle collisions. The diatomic nature of nitrogen means that molecular collisions will be inelastic and result in an energy exchange between the translational and rotational energy components. The Larsen-Borgnakke energy exchange model [1] has been activated to account for this.

A mesh of 100 × 60 cells was used and the time-step chosen was 4×10^{-6} s. The total number of DSMC particles in the system at steady-state was 327,000 and the cpu run-time was 4 hours using a single P4, 2.3 GHz chip.

Time averaging of the instantaneous DSMC particle fields was performed once steady-state had been achieved. The solution was considered to be steady when the total DSMC particle population and the average linear kinetic energy of the system showed only small changes with time. An example of this is shown in Figure 3.

Figure 4 shows a comparison with temperature and Mach number contours determined with Bird's DS2V code [1]. The local skin friction coefficient, C_f, and local heat transfer coefficient, C_h, distributions along the plate are show in Figure 5, where C_f and C_h are defined as follows:

$$C_f = \frac{F_d}{\frac{1}{2}\rho U^2} \tag{4}$$

$$C_h = \frac{q}{\frac{1}{2}\rho U^3} \tag{5}$$

with F_d the drag force per unit area, q the normal heat flux, ρ the freestream density and U the freestream velocity. Finally, figure 6 shows the non-equilibrium velocity-slip and temperature- jump occurring on the plate surface. All of these figures show that *dsmcFoam* is in very good agreement with the standard Bird code.

4.3 Benchmark Case C : Non-Uniform 2D Hypersonic Flow over a Flat Plate

DSMC can usefully simulate wind tunnel tests of rarefied supersonic flow over a flat plate. The wind tunnel tests use planar laser induced fluorescence (PLIF) of seeded iodine within a free jet expansion of nitrogen to measure the boundary layer flow characteristics [19].

A numerical mesh of 120 x 80 cells was employed covering a domain size of 20 mm in the flow direction and 8 mm in the vertical direction. The boundary conditions for the first 2 mm in front of the leading edge of the plate were assumed to be specular while the plate surface was diffuse. The global Knudsen number (for a plate length of 20mm) is 0.004. The time-step was set to 1×10^{-7} s and the total number of DSMC particles in the system at steady-state was 342,000. The non-uniform inflow conditions for this DSMC simulation are shown in figure 7; *dsmcFoam* straightforwardly handles non-uniform distributions for the inlet conditions of velocity, temperature and number density.

Figure 8 shows the resulting velocity profiles in the boundary layer at x =10 mm; the *dsmcFoam* solution is compared with the solution using the MONACO DSMC code [20,21] together with the PLIF experimental data [19]. There is reasonable agreement between *dsmcFoam* and the published data.

4.4 Benchmark Case D : 2D Hypersonic Flow Over a Cylinder

This case considers the Mach 10 cross flow of argon over a 12-inch diameter cylinder. This case was considered as a benchmark trial for several DSMC codes at the workshop DSMC '07 [12,22]. The inlet flow stream temperature is 200 K while the surface temperature of the cylinder is 500 K. The freestream number density is 4.247×10^{20} atoms/m^3 and the Knudsen number based on the cylinder diameter is Kn = 0.01. 1.3 million DSMC simulator particles were used and a time step of 1.5×10^{-8} s employed. Freestream boundaries exist at the inlet and outlet of the domain and symmetry conditions are employed at the centre-line. The VHS collision model was used and the cylinder had diffusive wall boundaries with full thermal and momentum accommodation. Cyclic (periodic) conditions were applied on all other boundaries. The overall solution time using a single Pentium IV - 3 GHz chip was 36 hours.

Figure 9 shows the contours of Mach number alongside the results of the same case calculated using the industry-standard DS2V code of Bird [1]. Figure 10 shows the heat flux around the cylinder predicted by *dsmcFoam* and Bird's DS2V code. The profiles predicted by both codes appear to be in good agreement, although *dsmcFoam* does predict a somewhat higher maximum heat flux at the stagnation point. Further studies of *dsmcFoam* grid, particle number and time-step sensitivity are necessary in order to provide a conclusive result for the heat flux distribution.

Figure 11 shows the velocity-slip and temperature jump contours along the cylinder for the case of Ma = 10 and Kn = 0.25. The *dsmcFoam* results are compared with the predictions of Lofhtouse [22] using the MONACO DSMC code. There is reasonable agreement between *dsmcFoam* and the Lofthouse data although some statistical scatter is observed in the *dsmcFoam* results in the highly rarefied wake region of the cylinder.

4.5 Benchmark Case E : 3D Hypersonic Corner Flow

This case is the hypersonic flow of nitrogen through a 3D corner and is another benchmark case of Bird [1]. The flow domain consists of two adjacent walls, connected at 90^{o} to each other with the surfaces opposite to these walls being freestream. In a similar manner to the flat plate case C, symmetry conditions are applied for a short length upstream of the leading edges of the walls.

The Mach number is 6 and Knudsen number 0.043. The walls are diffuse with a temperature of 1000 K and all other boundaries are freestream at a temperature of 300 K. There are 1×10^{20} molecules/m^3, VHS collisions apply and the Larsen-Borgnakke energy redistribution model is activated. The time step size was 1×10^{-6} s.

In order to compare directly with the same case in Bird's book an identical number of computational cells have been used, namely, 30 × 18 × 18. The *dsmcFoam* case was run in parallel using 4 cpus (Pentium-IV, 3 GHz) and the run-time was 5 hours.

Figures 12 and 13 show a comparison between results from *dsmcFoam* and from Bird's code for the wall skin friction and heat transfer coefficients, C_f and C_h, respectively. In both cases the contour plots show a very good qualitative concurrence between the Bird results and *dsmcFoam*. Figures 14-16 show the results for four different cross-sections of the flow. The plots are for Mach number, dimensionless density and dimensionless temperature respectively. In all cases the contour plots show excellent agreement between *dsmcFoam* predictions and the Bird results.

4.6 Benchmark Case F : 3D Hypersonic Flow over a Flat-Nosed Cylinder

Although this case has been considered by Bird [1] as a 2D axisymmetric problem, *dsmcFoam* does not currently have an axisymmetric capability. However, the case may be run as a 3D, quarter-section model with symmetry boundary conditions. Use was also made of the OpenFOAM meshing utility *snappyHexMesh*, which creates a 3D mesh by 'snapping' a regular, hexahedral mesh on to the surface of a complex geometry where the geometry is in *stl* format. Figure 17 shows the unstructured mesh around the cylinder.

The case considers the flow of argon at a number density of 1×10^{21} atoms/m^3 and a temperature of 100 K at a velocity of 1000 m/s over a flat-nosed cylinder. The radius of the cylinder is 0.01 m so that the Knudsen number based on the diameter of the cylinder is 0.0474. The Mach number of the flow is 5.37 and the surface temperature of the cylinder 300 K. The cylinder walls were set as diffuse.

275,000 computational cells were created following the grid-snap, and 24 simulator particles per cell were used to initialise the flow field. The time-step size was 1.87×10^{-7} s and at steady-state there were 8.37 million DSMC particles in the system. The cpu run time was 31 hours running in parallel with 6 processors (Pentium IV, 3 GHz). Scalability trails using 6 processors showed a speed up factor of 4 compared with a single processor.

Figure 18 shows the dimensionless number density contours in a 3D plot around the quarter-cylinder section. Other results for the non-dimensional density and temperature are shown in figures 19 and 20. The shock layer has been well-captured and, in comparison with the results from Bird's DSMC2A code, the *dsmcFoam* results once again show very good agreement.

The parallel processing capability of *dsmcFoam* within OpenFOAM is an attractive feature considering the substantial numerical resources normally required to obtain practical DSMC solutions. Both multi-core workstations and high performance computing (HPC) architectures can take advantage of the limitless parallel decomposition opportunities within OpenFOAM.

5. Comments and Future Work

We have presented benchmark trials of a new, open source DSMC code called *dsmcFoam*. The code has been written within the framework of the open source CFD toolbox OpenFOAM. Distinguishing features of the *dsmcFoam* code include its modular C++ construction with easy implementation of new user coding, unlimited parallel processing capabilities and an ability to handle complex, 3D geometries.

Results for the initial benchmark trials show very good agreement with analytical solutions and the industry-standard code developed by Graham Bird. Parallel scalability tests showed a speed-up of 4 when using 6 cpus, which could probably be improved upon with better cpu load balancing.

Short term future work for *dsmcFoam* will include the implementation of more sophisticated collision models (e.g. VSS), the inclusion of vibrational energy exchange leading to chemically reacting flows and the implementation of pressure-driven boundary conditions for low-speed, rarefied gas flows. Longer term objectives may include transient adaptive schemes in space and time.

Practical solutions for rarefied gas flows exhibiting non-equilibrium and non-continuum physics necessitate a DSMC approach. The engineering problems that DSMC is therefore appropriate for range from civilian hypersonic vehicles to micro gas fuel cells for portable electronic devices. The accessibility and functionality of the *dsmcFoam* code means that it can reach a wider scientific audience beyond the current DSMC community; open source codes represent a collective effort to provide freely accessible, useful resources for the benefit of all users. It is therefore hoped that any users making future advances with the *dsmcFoam* code will quickly disseminate their work and make the additional coding and models freely available for use by others.

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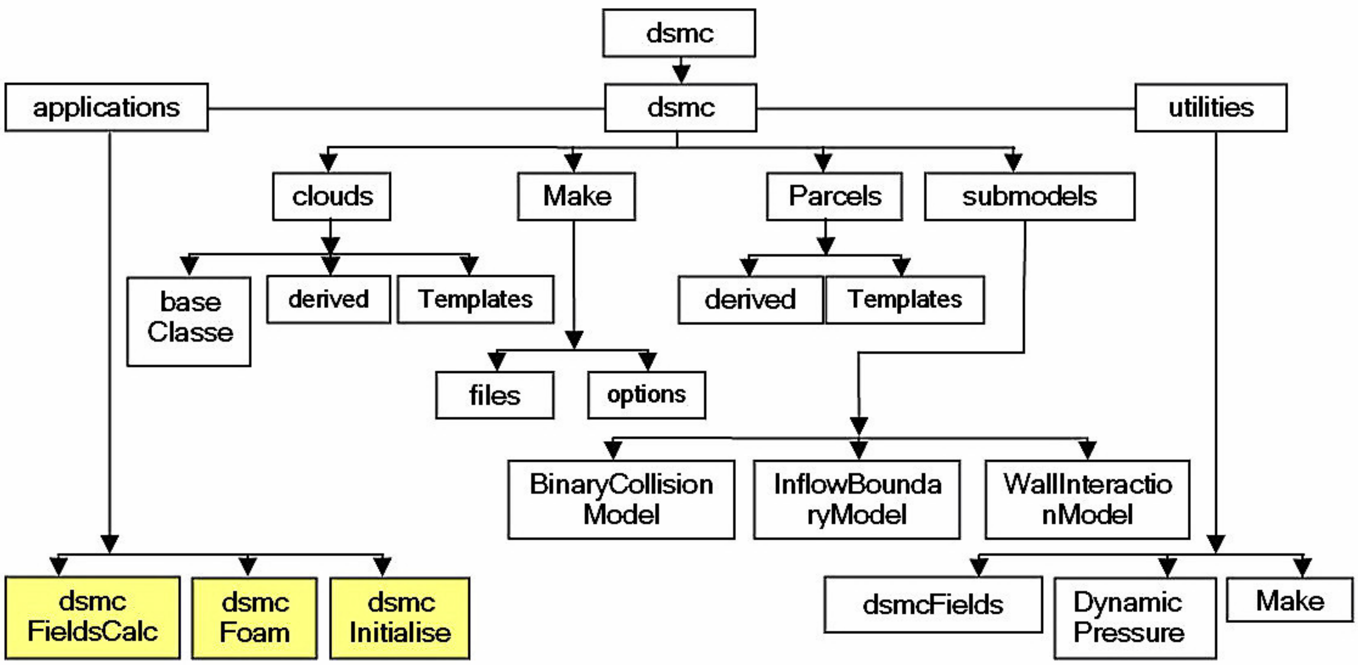


Figure 1 *Directory structure of dsmcFoam*.

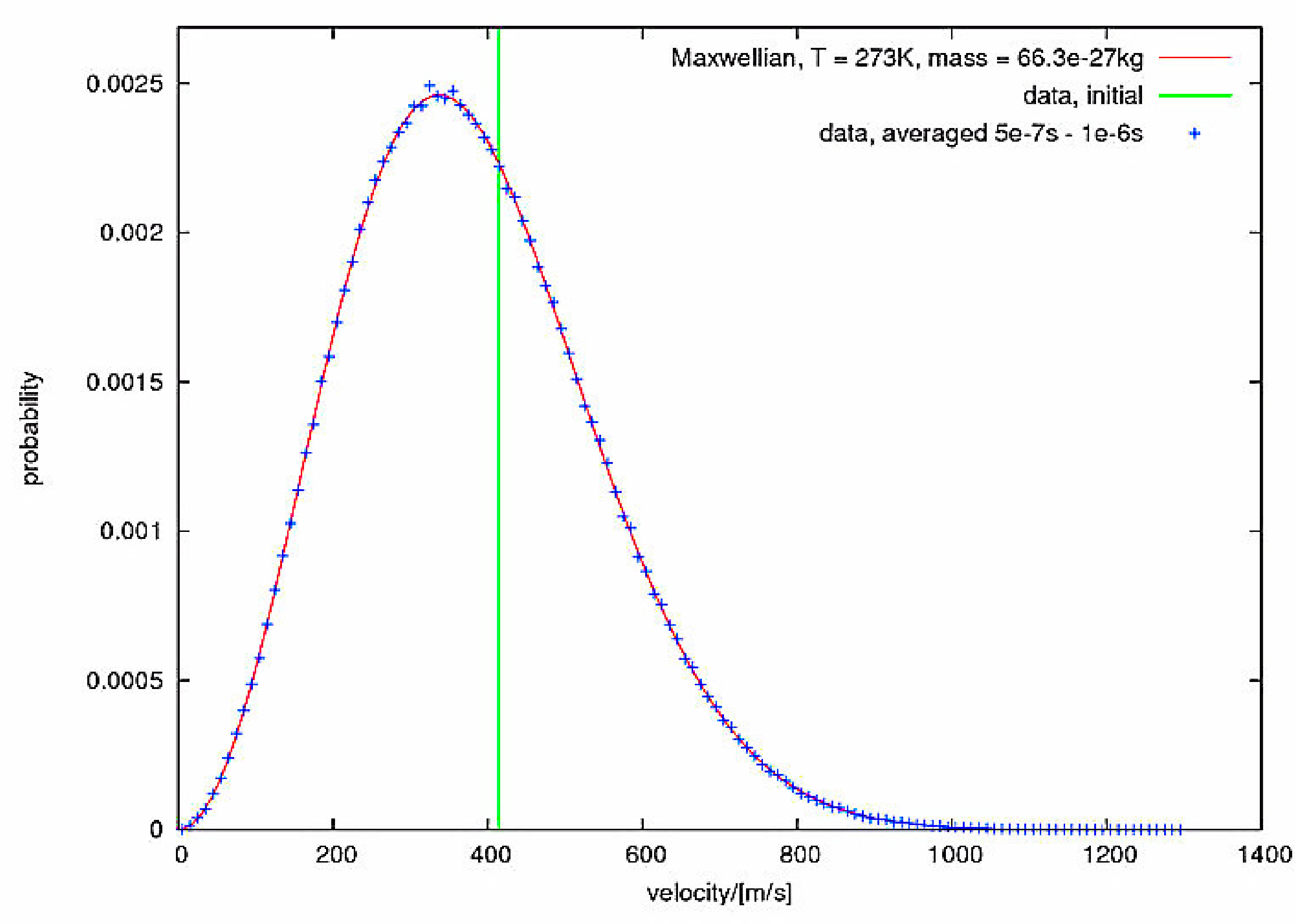


Figure 2 *Relaxation to equilibrium, Case A*.

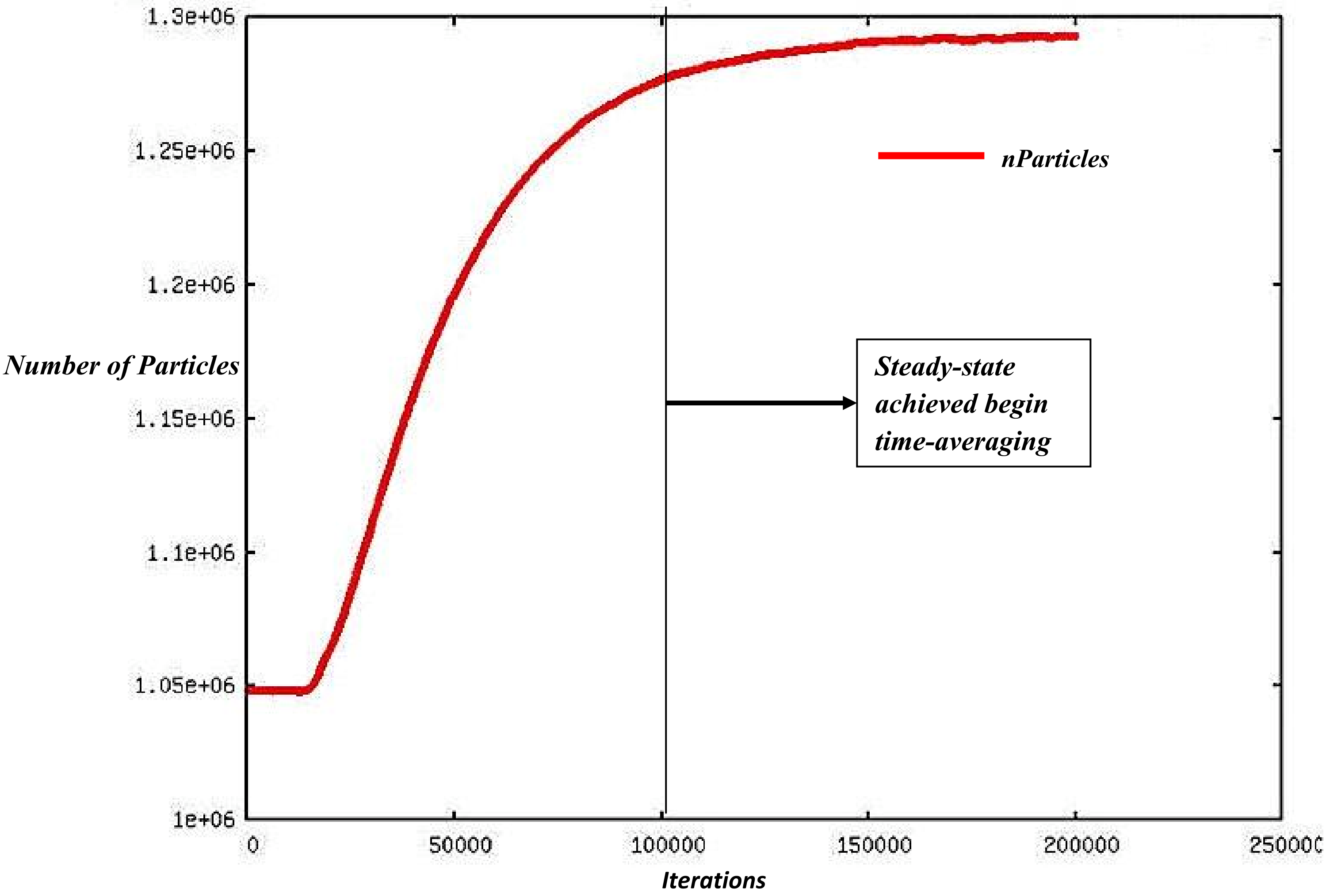


Figure 3 *Example of estimation of steady-state conditions*.

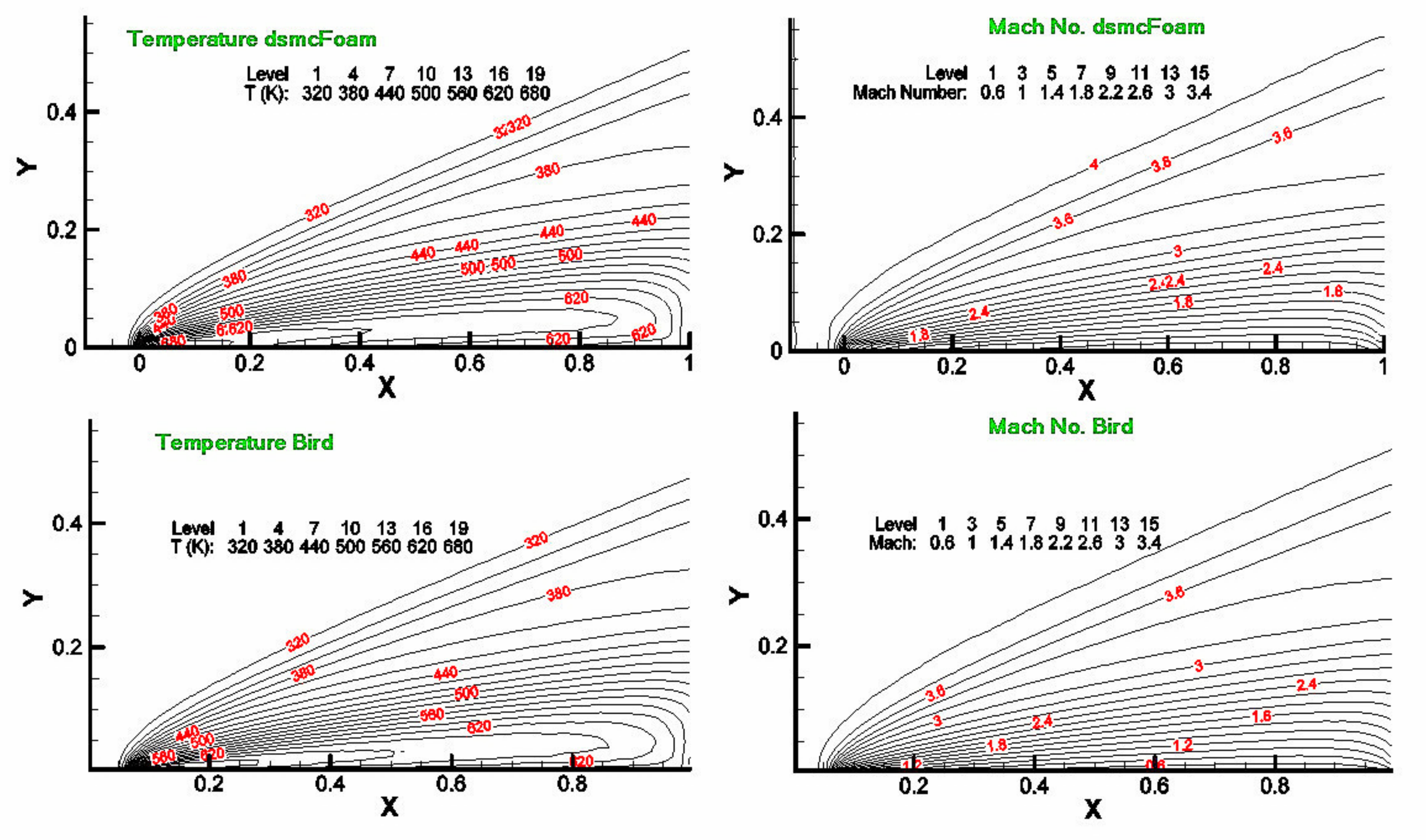


Figure 4 *Comparison of temperature and Mach number contours along the 2D flat plate of Case B. The upper figures are output from dsmcFoam, the lower figures from Birds' DS2V code.*

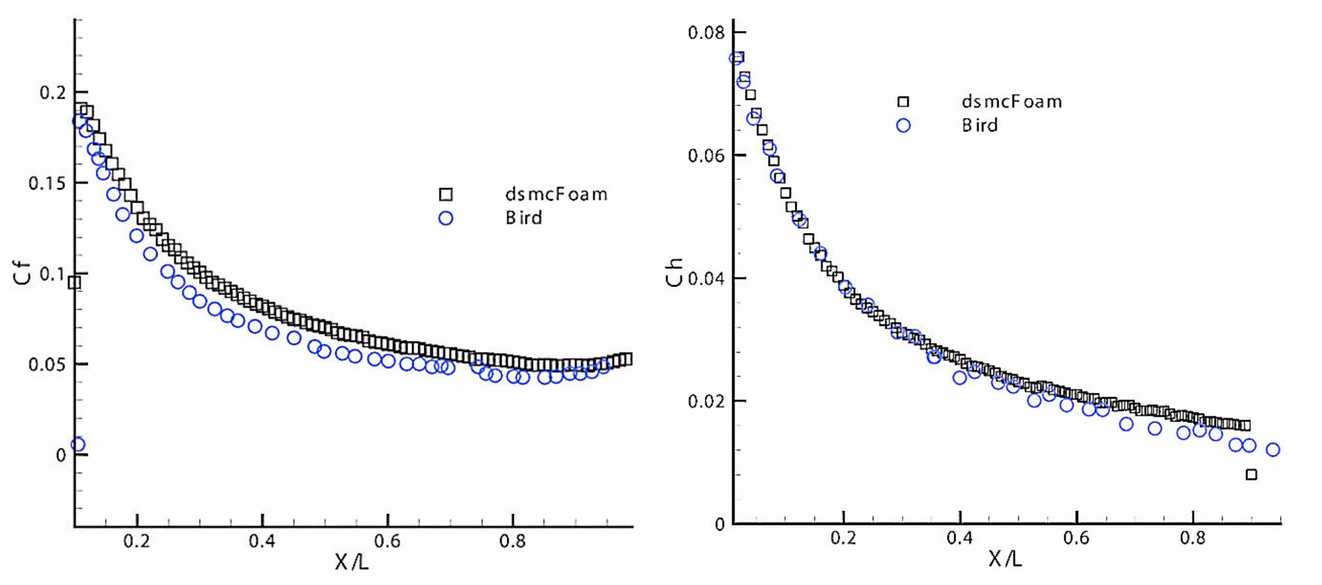


Figure 5 *Comparison of different DSMC code calculations of the skin friction coefficient C_f and heat transfer coefficient C_h along the 2D flat plate of Case B*.

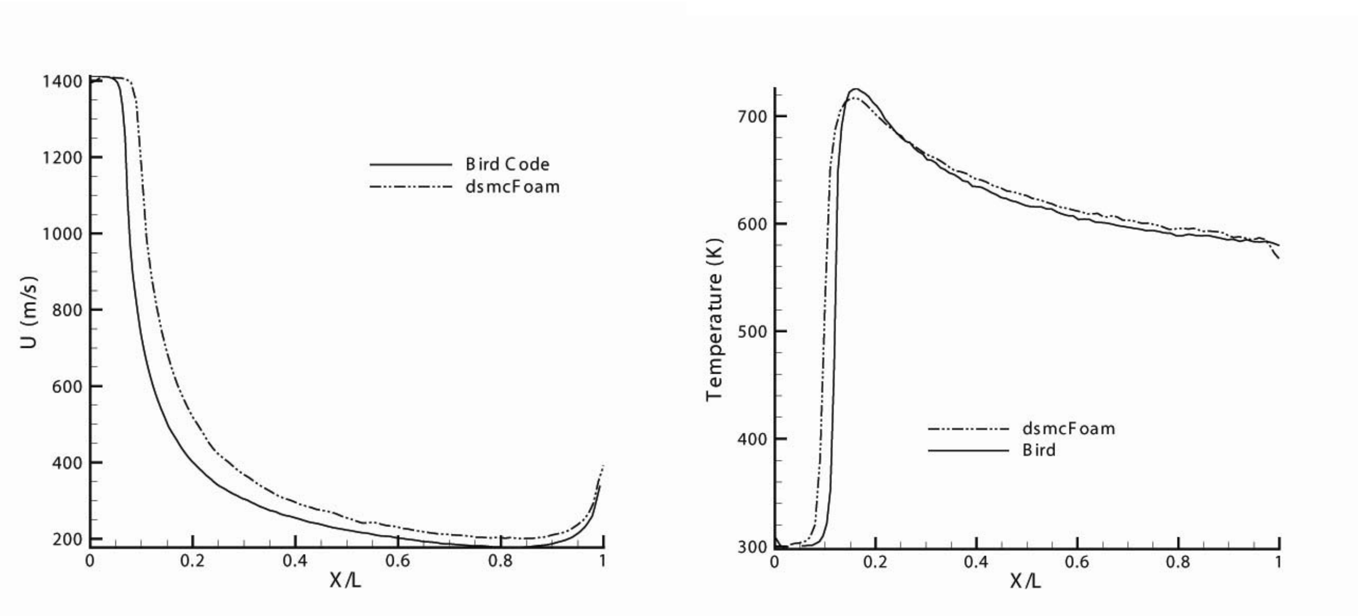
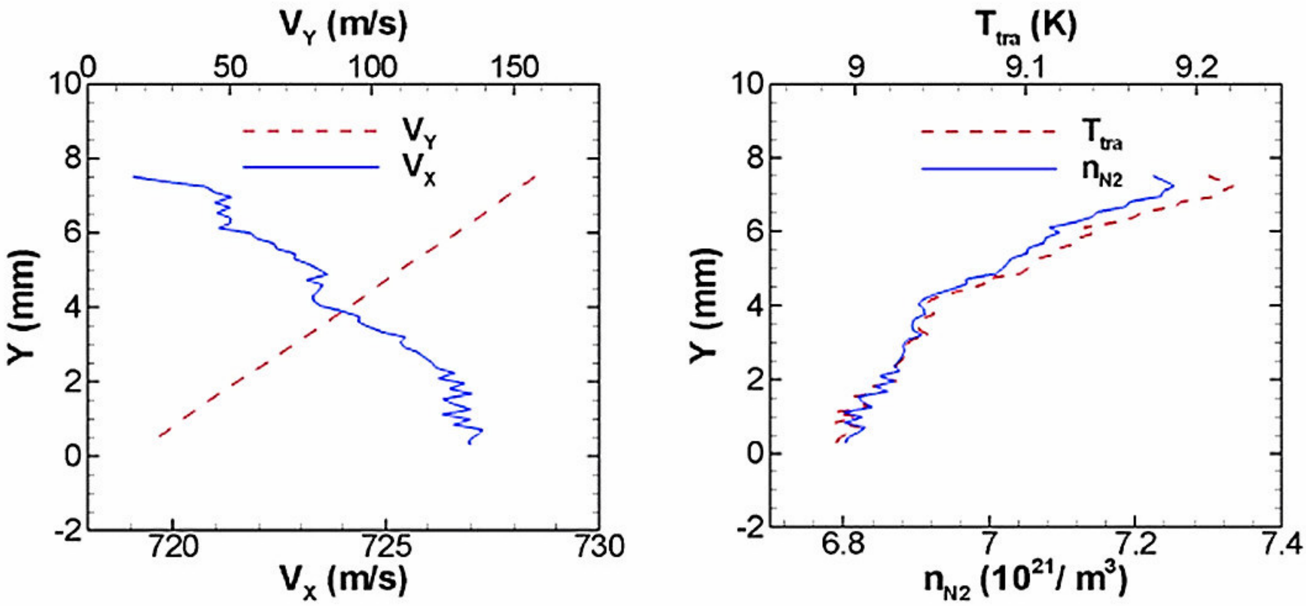
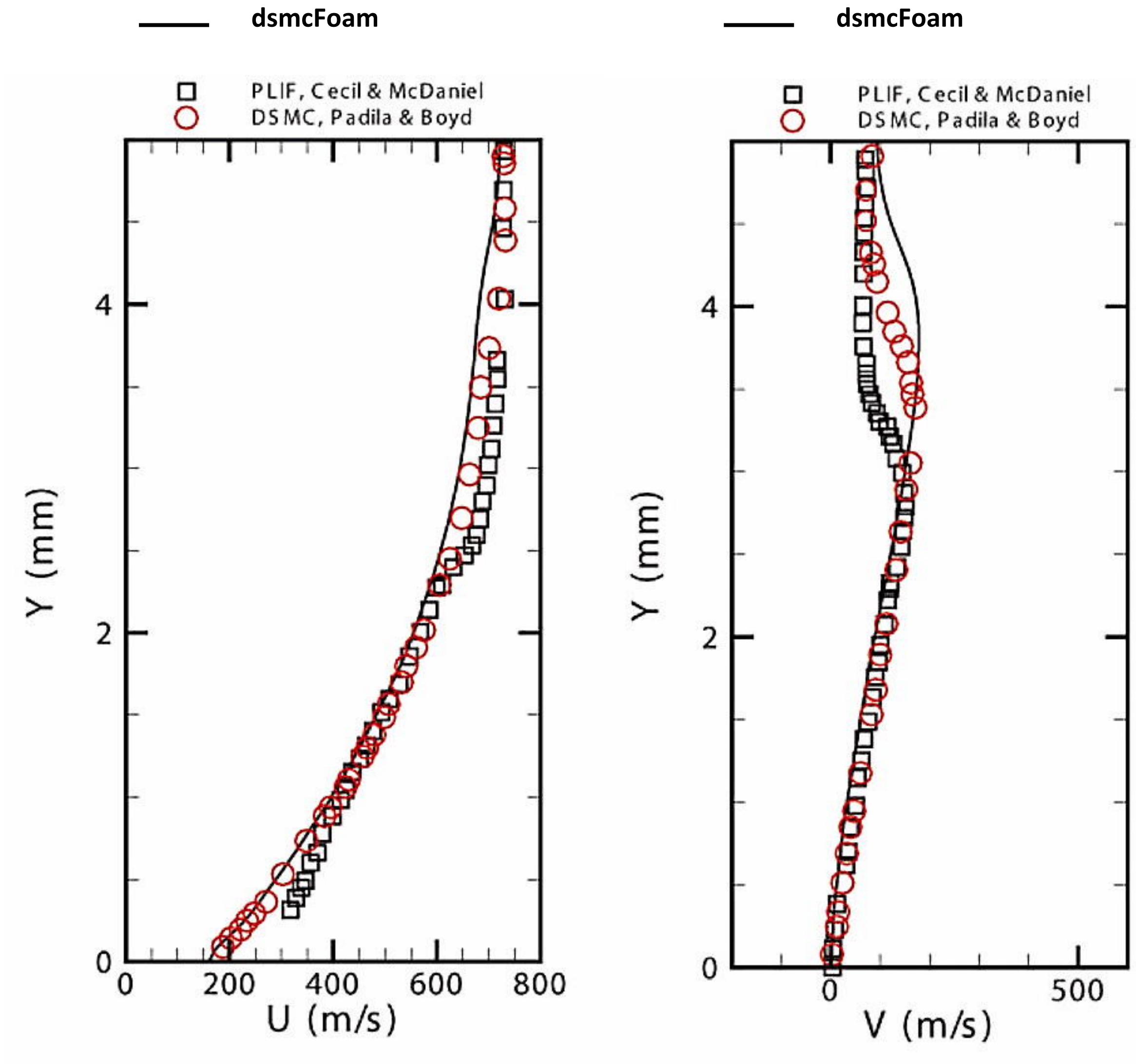


Figure 6 *Comparison of calculated velocity-slips and temperature-jumps along the 2D flat plate of Case B*.



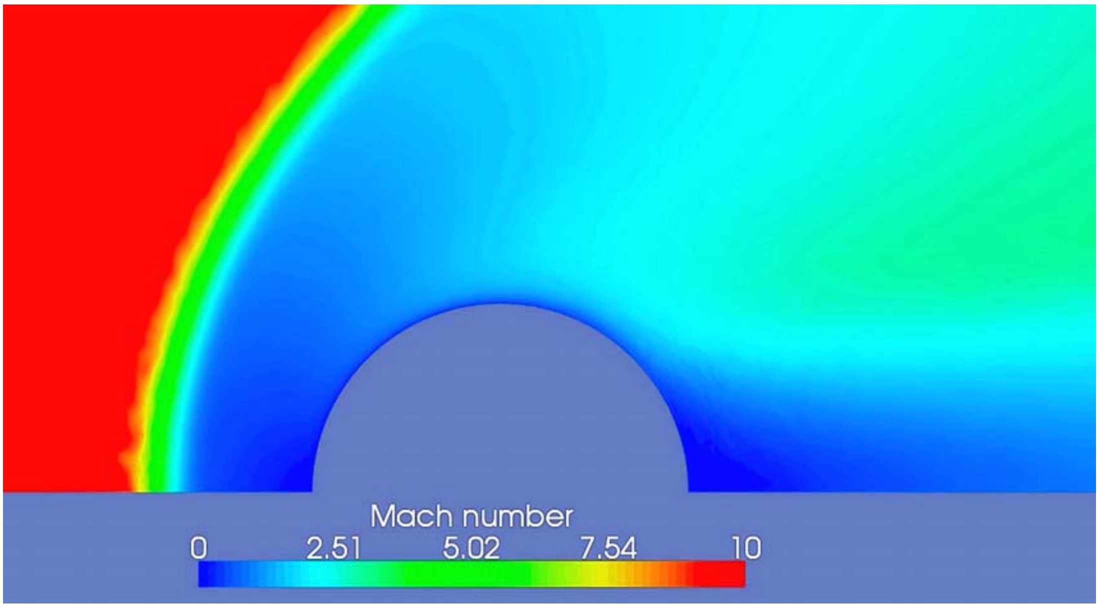
(a) *Velocity*　　　(b) *Temperature and number density*

Figure 7 *Non-uniform inlet conditions for Case C, hypersonic nitrogen flow over a flat plate*

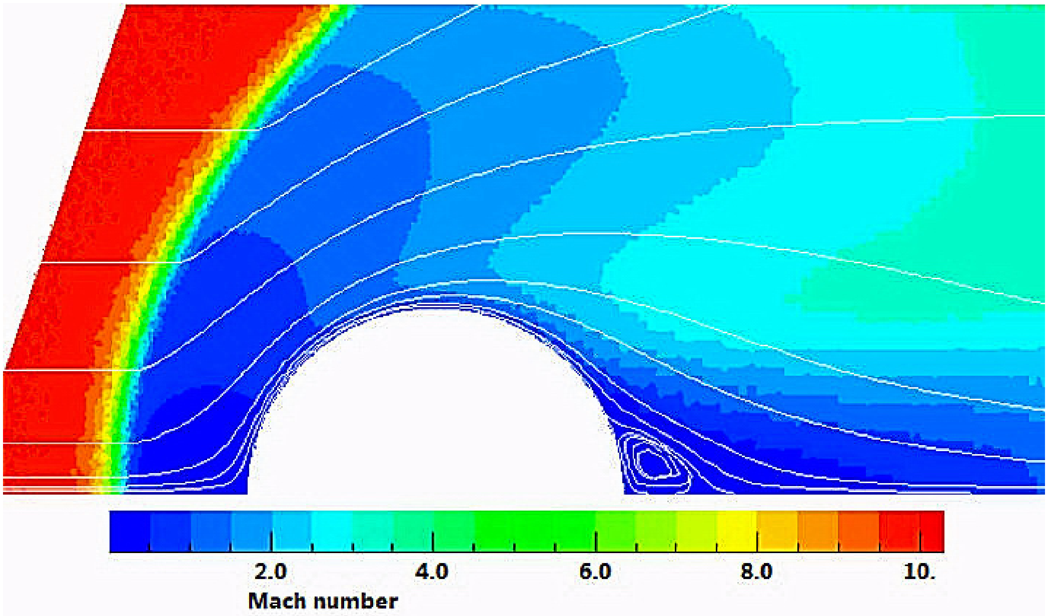


(a) *x-component velocity* (b) *y-component velocity*

Figure 8 *Boundary layer profiles at x = 10 mm for Case C, hypersonic nitrogen flow over a flat plate*.

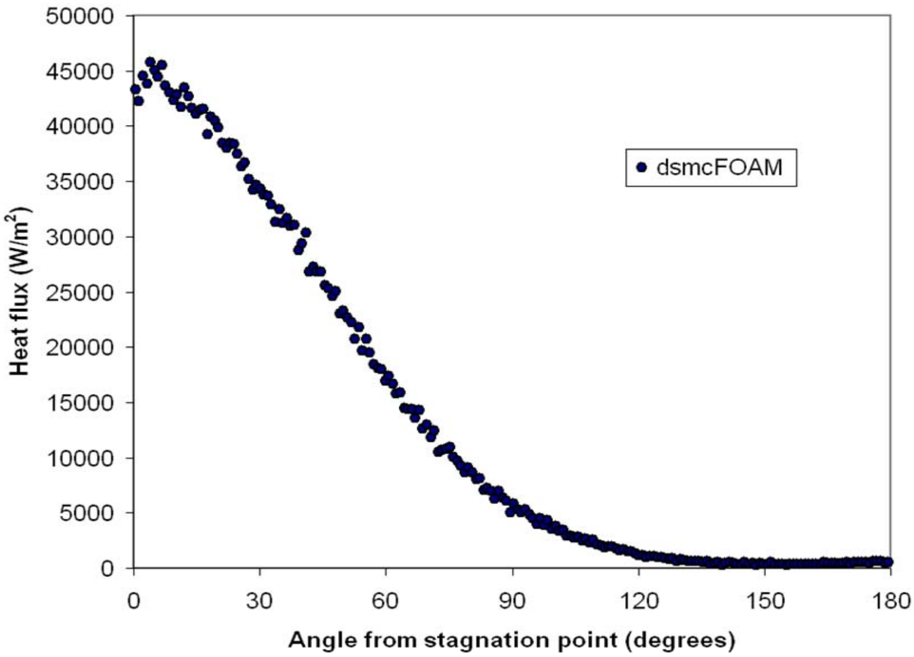


(a) *dsmcFoam*

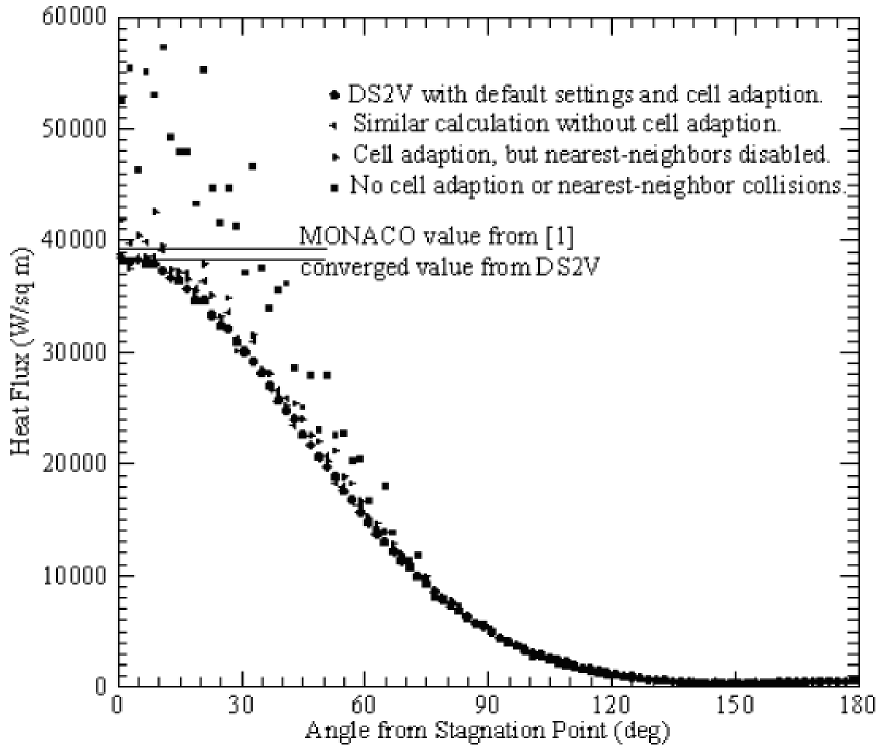


(b) *DS2V*

Figure 9 *Calculated Mach number contours for Case D, 2D hypersonic flow over a cylinder, $Ma = 10$, $Kn = 0.01$.*



(a) *dsmcFoam*



(b) *DS2V*

Figure 10 *Predicted heat flux distributions around the cylinder in Case D.*

Ma = 10, Kn = 0.01.

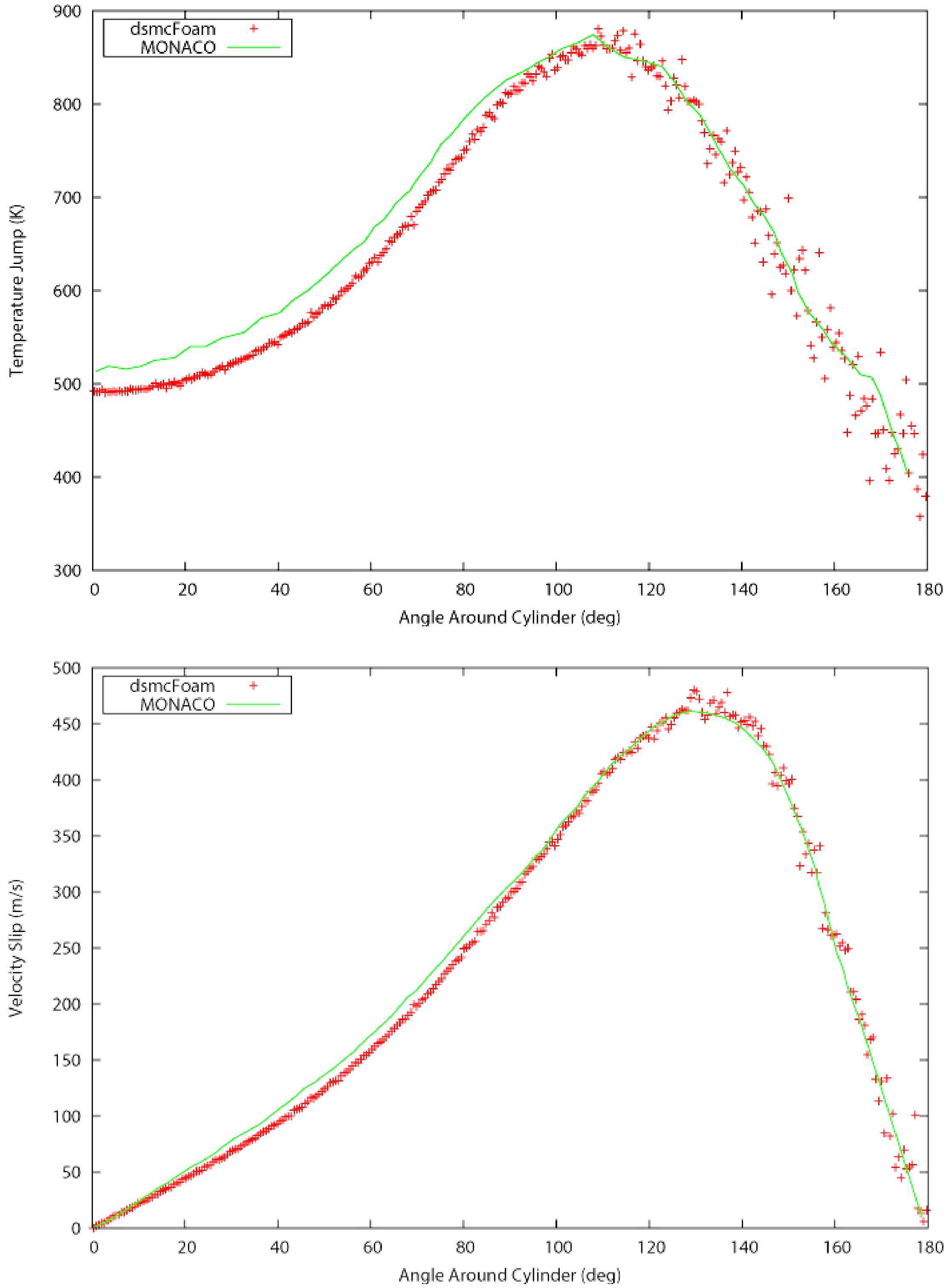
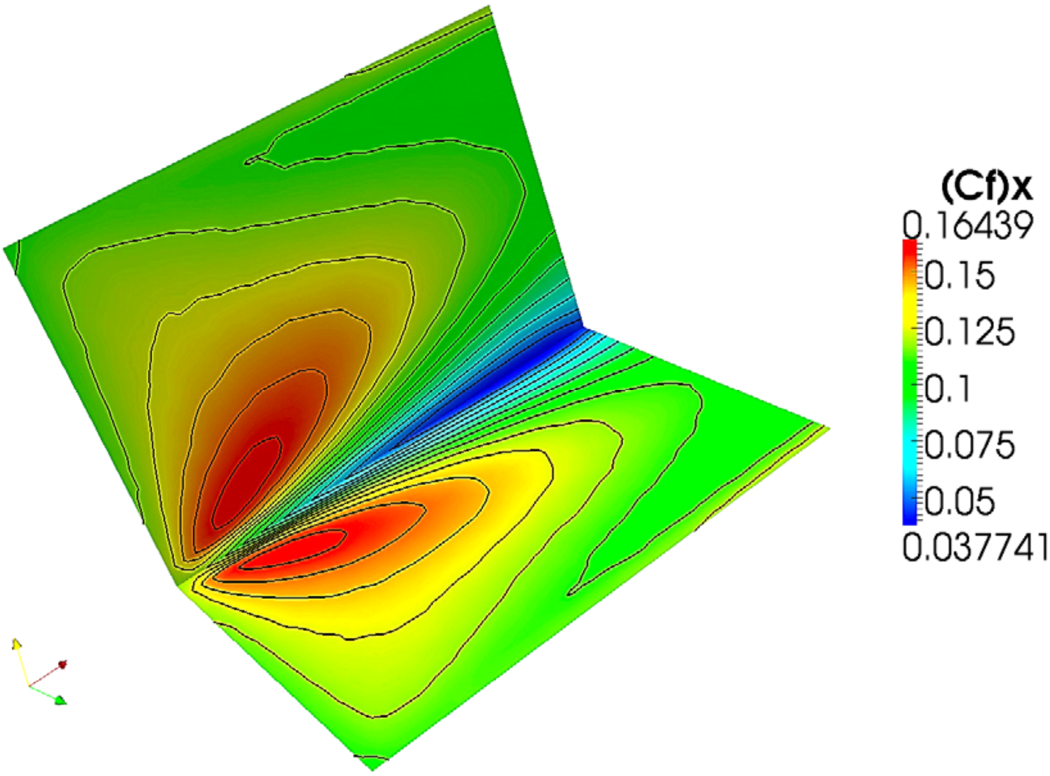
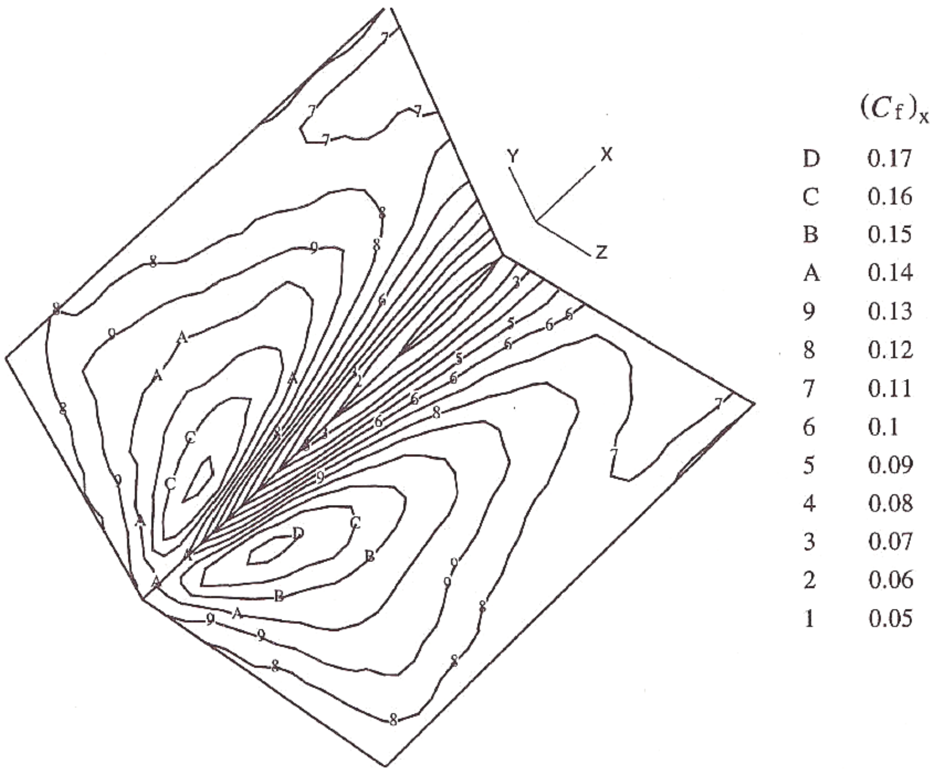


Figure 11 *Comparison of calculated velocity-slips and temperature-jumps along the cylinder in Case D, Ma = 10, Kn = 0.25*.

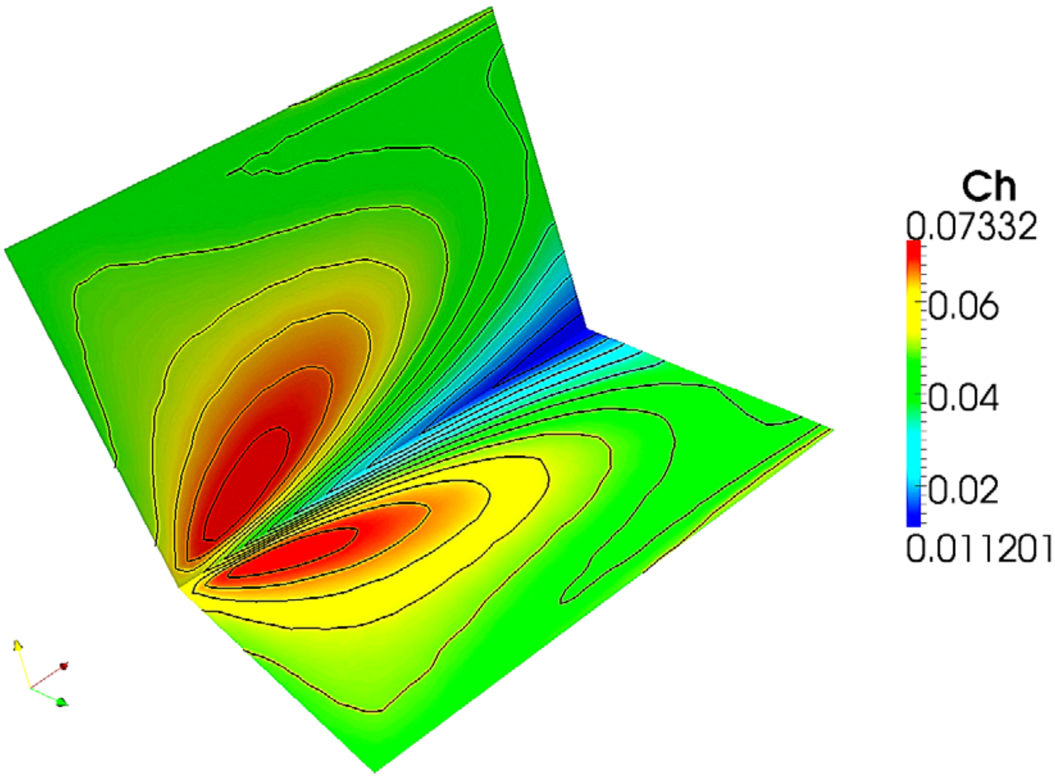


(a) *dsmcFoam*

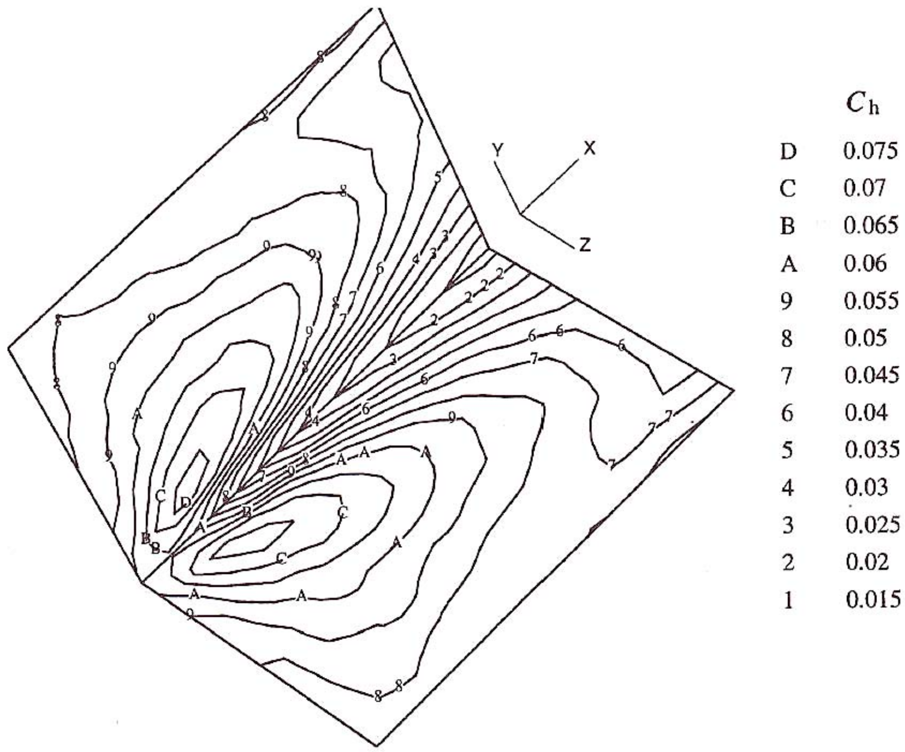


(a) *DS2V*

Figure 12 *Calculated skin friction coefficients* $(C_f)_x$ *for Case E, 3D hypersonic corner flow*.



(a) *dsmcFoam*



(a) *DS2V*

Figure 13 *Calculated heat transfer coefficients C_h for Case E, 3D hypersonic corner flow*.

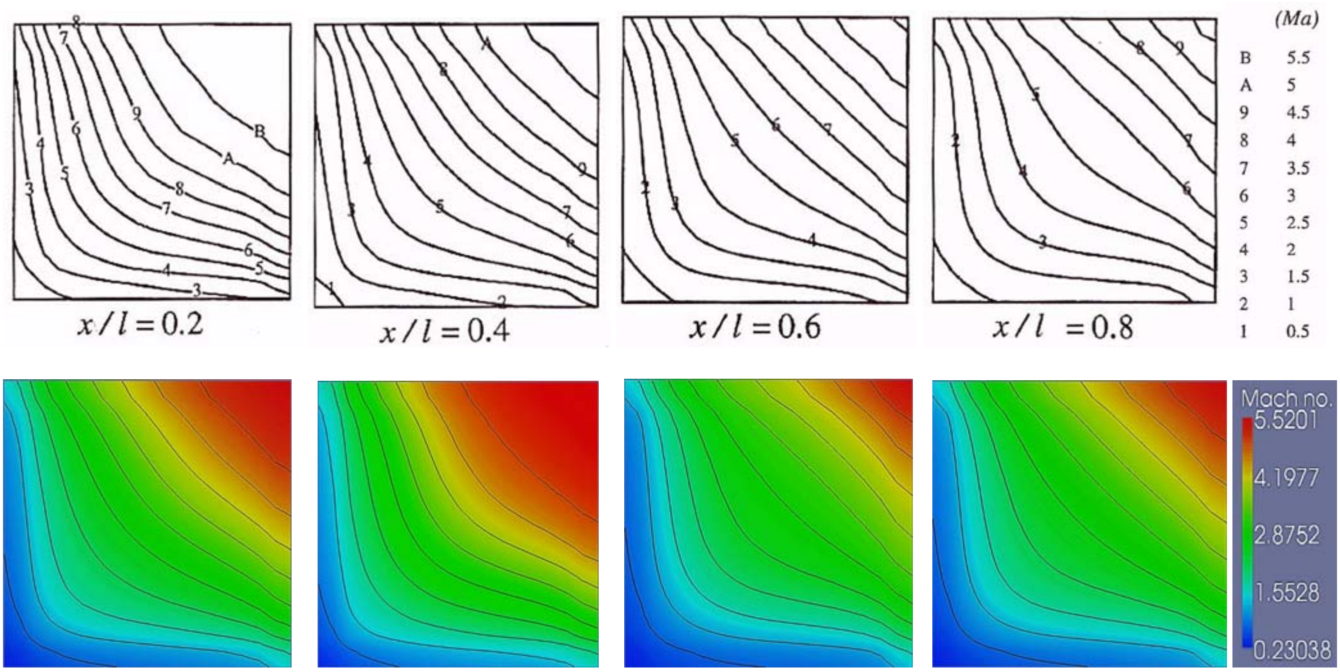


Figure 14 *Mach number contours for Case E, 3D hypersonic corner flow; DS2V* (top), *dsmcFoam* (bottom).

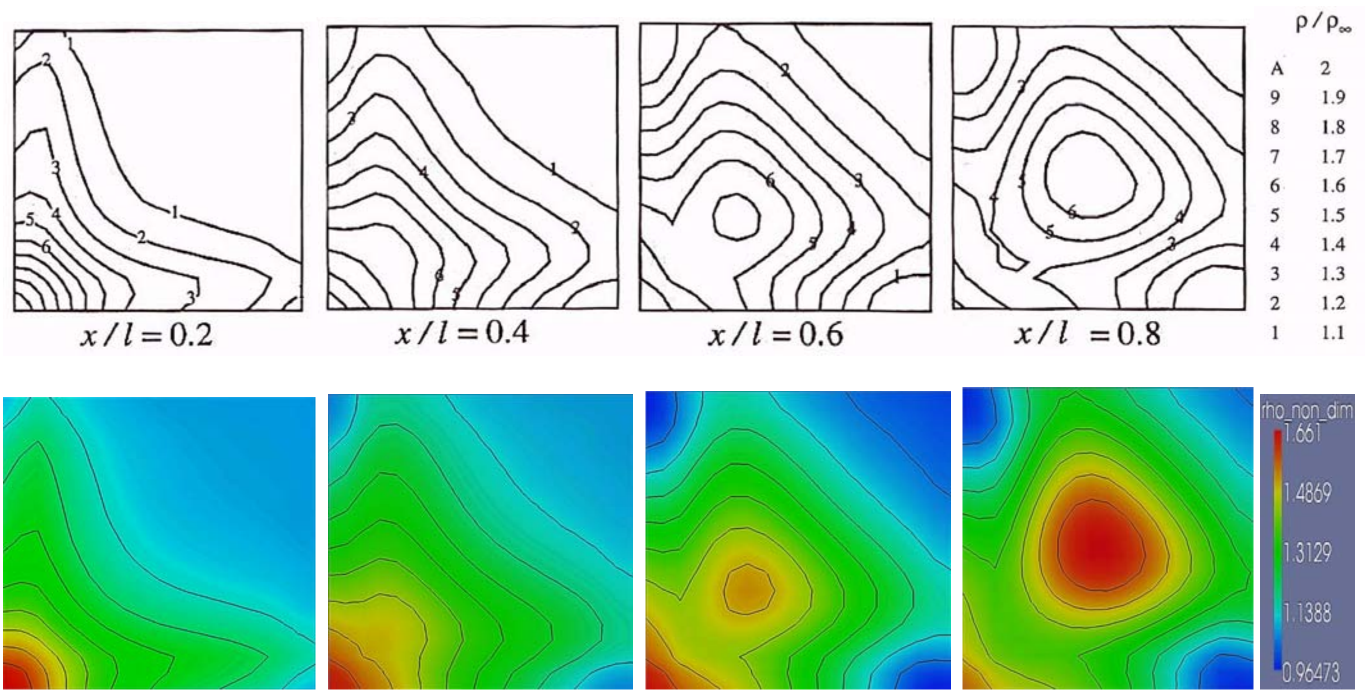


Figure 15 *Dimensionless density contours for Case E, 3D hypersonic corner flow; DS2V* (top), *dsmcFoam* (bottom).

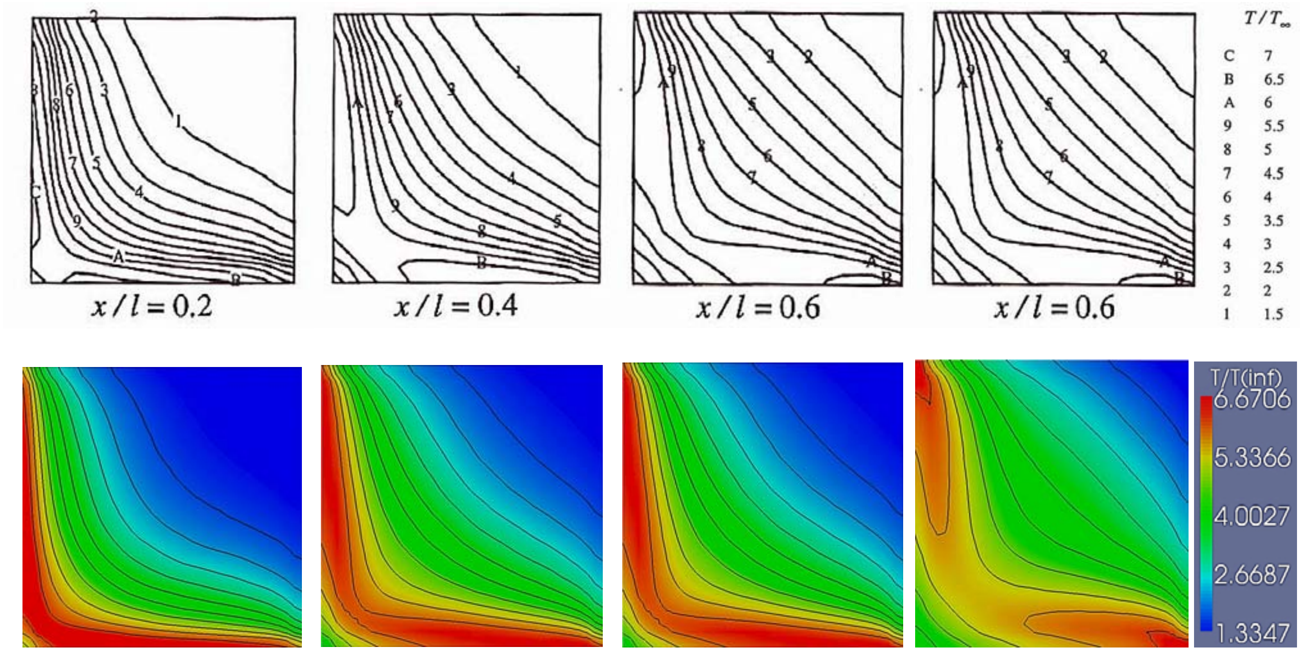


Figure 16 *Dimensionless temperature contours for Case E, 3D hypersonic corner flow; DS2V* (top), *dsmcFoam* (bottom).

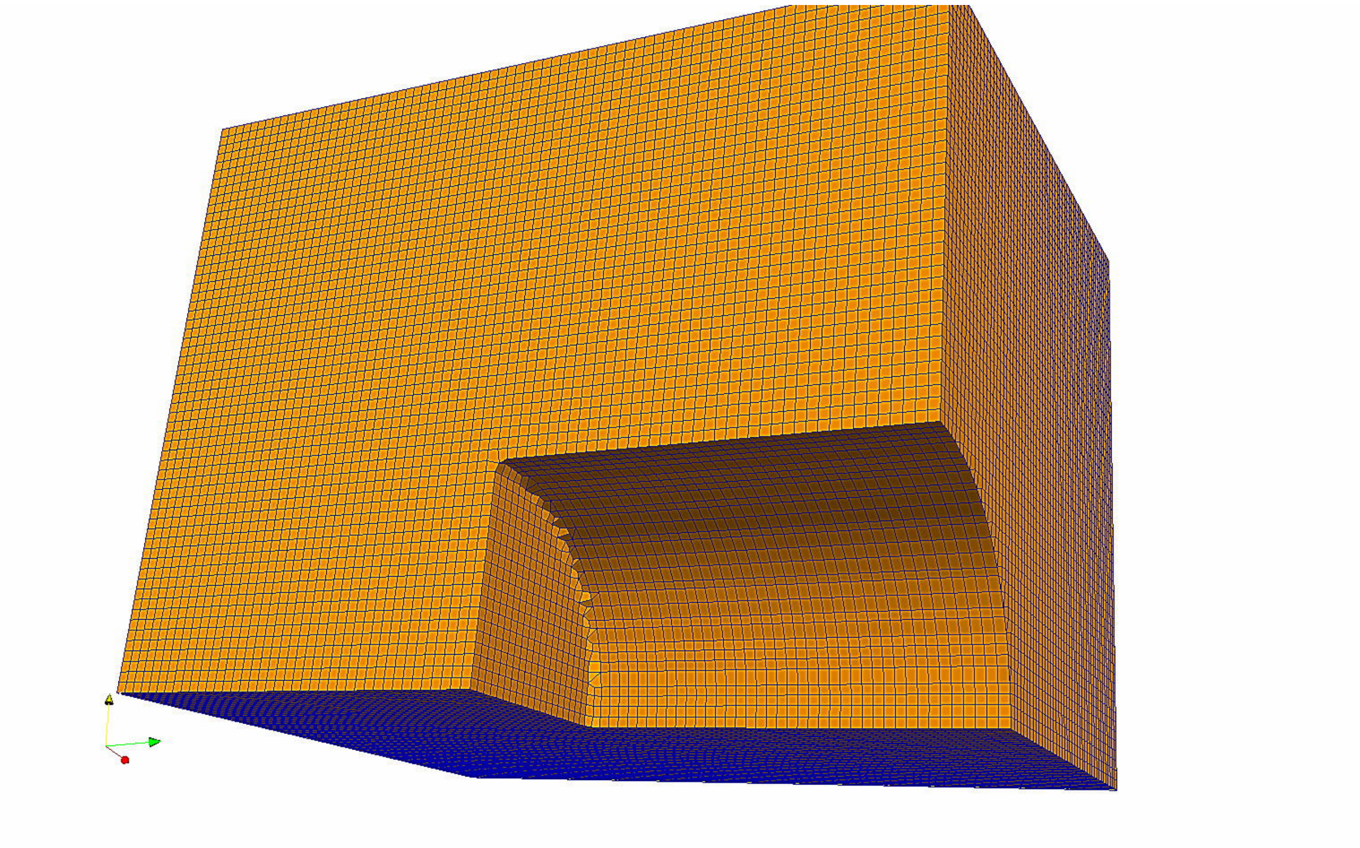


Figure 17 *Computational grid for Case F, 3D hypersonic flow over a flat-nosed cylinder*

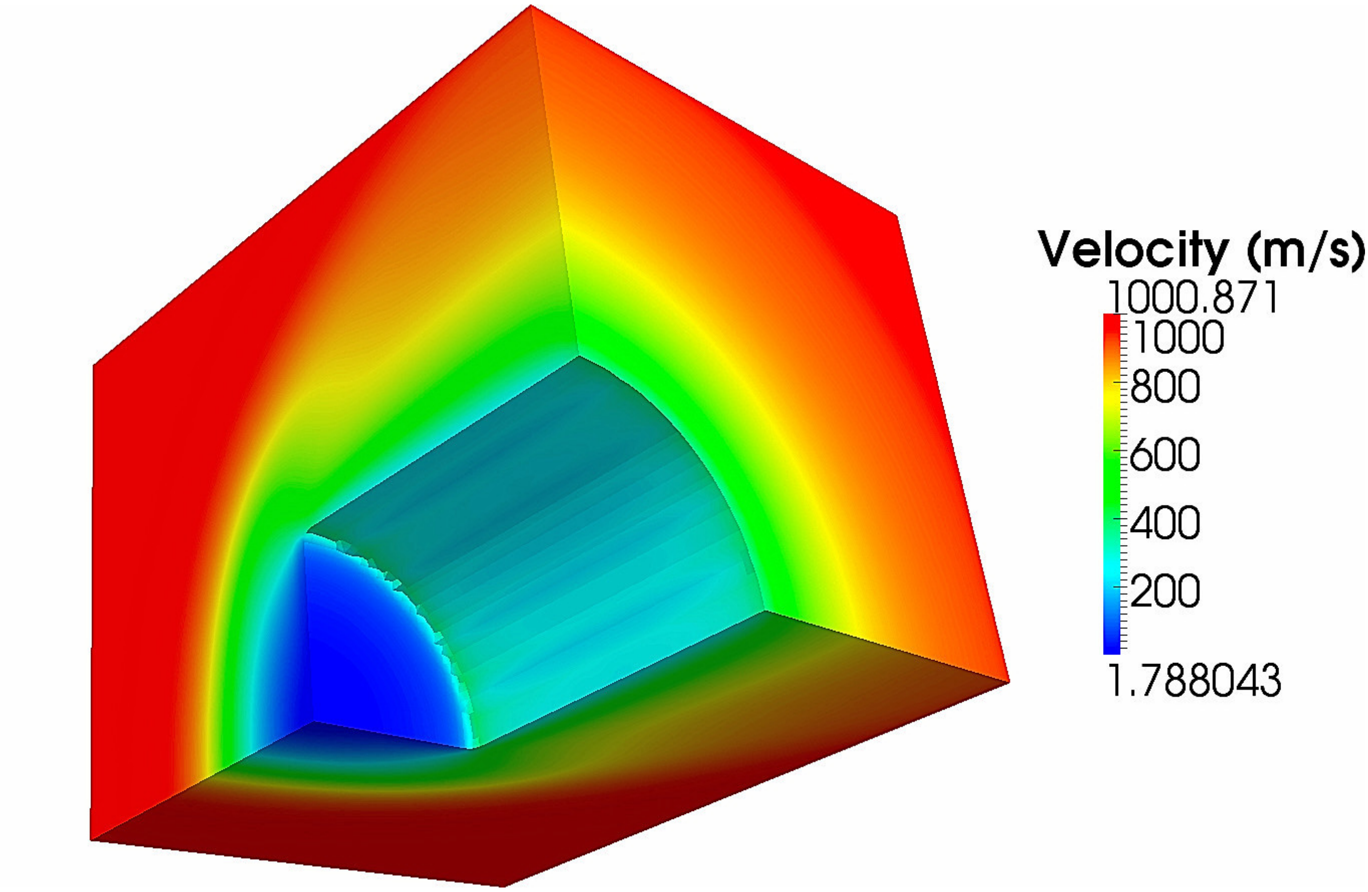
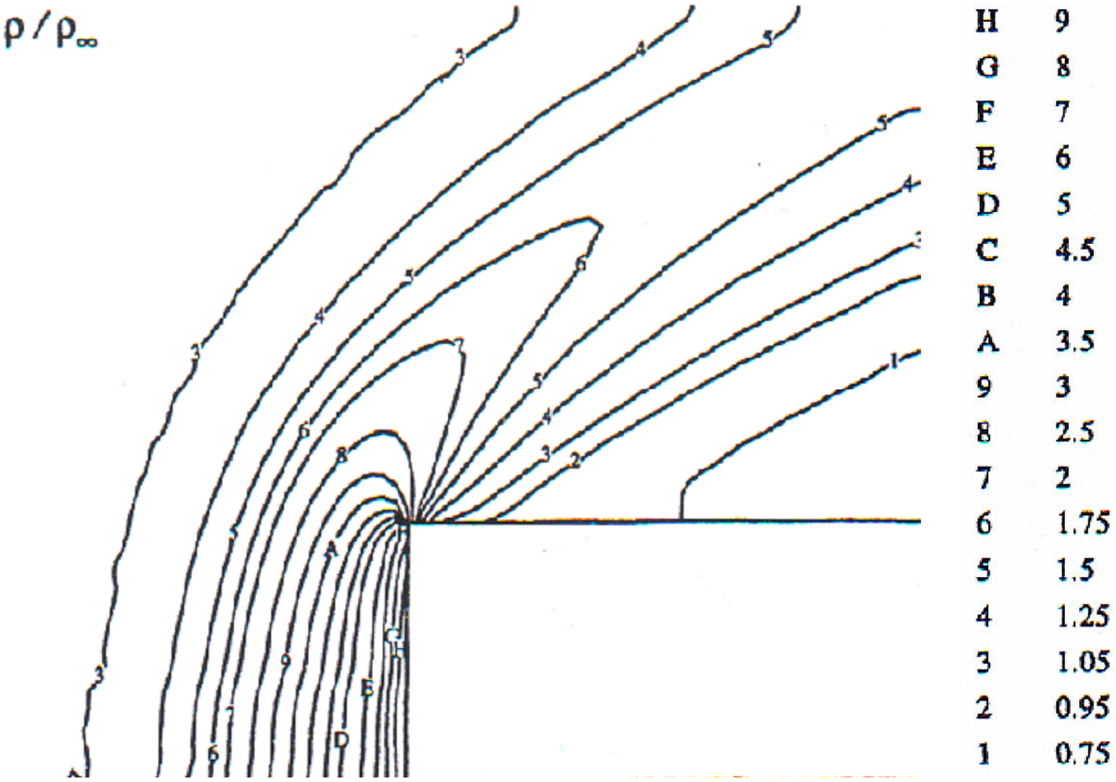
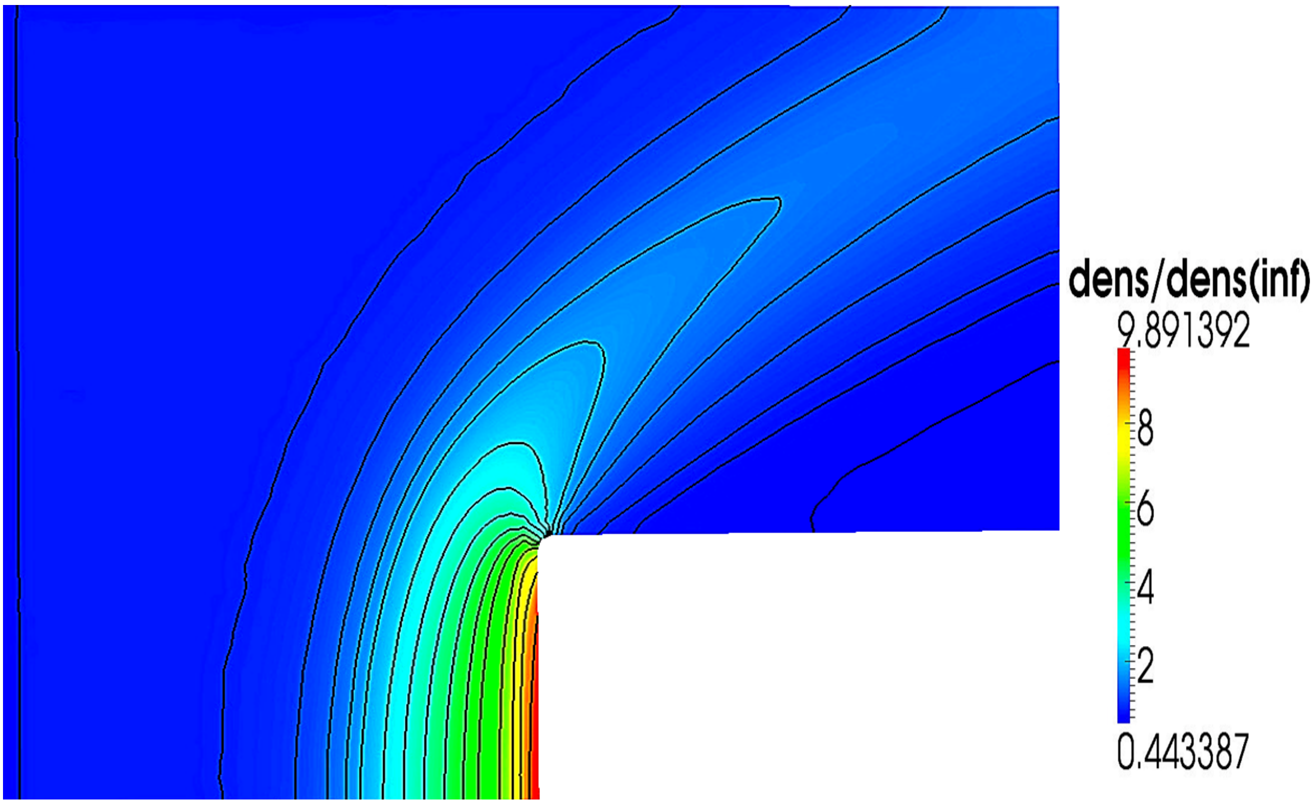


Figure 18 *dsmcFoam prediction of the velocity field for case F, 3D hypersonic flow over a flat-nosed cylinder*.

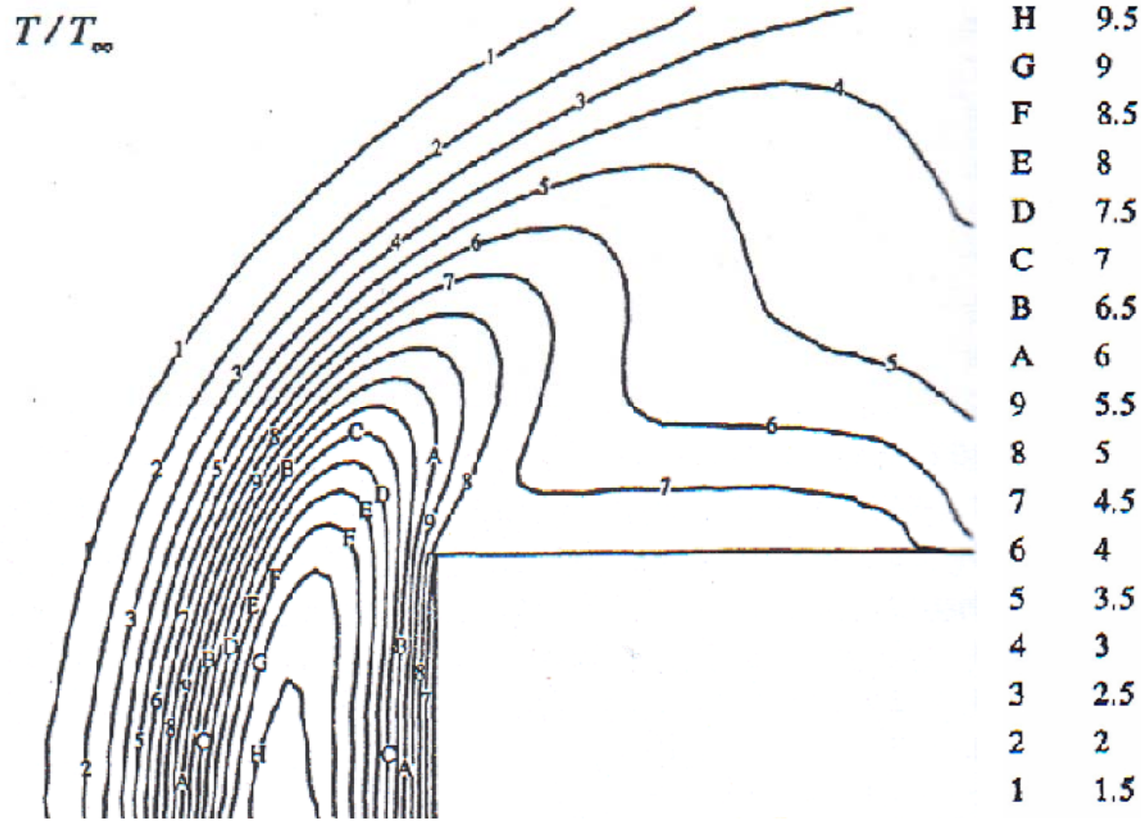


(a) *DS2VA*

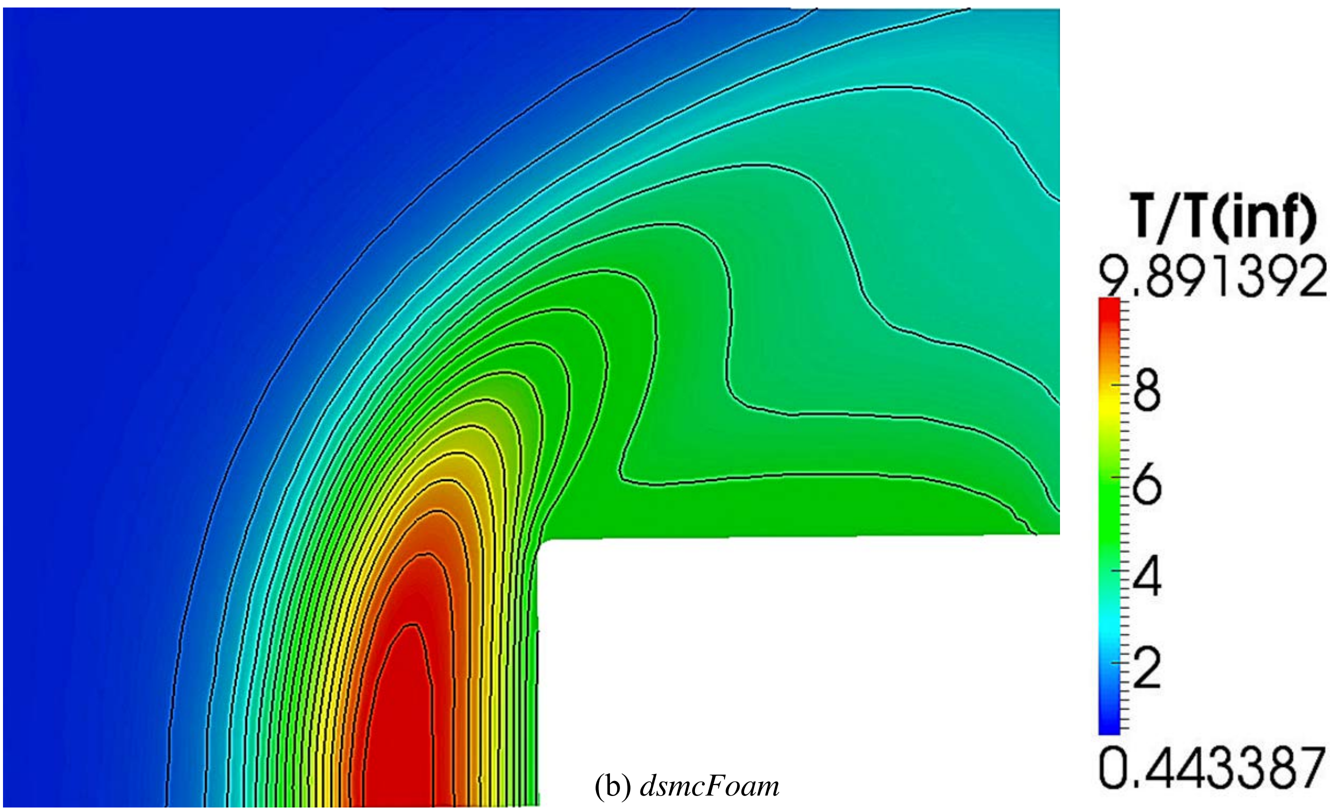


(b) *dsmcFoam*

Figure 19 *Contours of calculated dimensionless density for Case F, 3D hypersonic flow over a flat-nosed cylinder*.



(a) *DS2VA*



(b) *dsmcFoam*

Figure 20 Contours of dimensionless temperature for case F, 3D hypersonic flow over a flat-nosed cylinder.