

COMPUTATIONAL FLUID DYNAMICS AND COMPUTER AIDED DESIGN

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Abstract

Computational fluid dynamics based on the latest achievements of the mathematical models, numerical methods, novel algorithmic languages, operating systems with the last achievements in hardware. Recent advances in geometry modeling, surface and volume grid generation, computational algorithms have led to accurate predictions for increasingly complex and realistic configurations (aircraft, cars, ships, trains and etc.)

Aerodynamic design connected with research and development of methods, algorithms allowing determine the aerodynamic characteristics about bodies of the real form. Our researches are directed on studying of nonlinear effects and their influences on aerodynamic characteristics. The main problem is calculation of aerodynamic resistance (wave, friction, vortex), elevating and lateral forces, the center of pressure, the aerodynamic moments. The aerodynamic forces must be considered including aerodynamic damping, rotation concerning to an axis and a vector of speed. The developed methods allow define aerodynamic characteristics in wide ranges on a angle of attack and Mach number. The physical and chemical processes resulting in difference of gas properties from properties of perfect gas with a constant thermal capacity are taken into account.

Mathematical models

During the past decade a large number of computational codes have been developed that differ in the grid generation methods and numerical algorithms used. For numerical simulation of external flow fields past real form bodies it is necessary to construct the geometry, to design a discrete set-grid, to provide the mathematical model of the initial value problem, to approximate the governing equation by numerical ones, to design a computational algorithm, to realize the flow field, to establish a feed-back of obtained results with experiment, analytical and benchmark problems and so on.

As mathematical model the Navier-Stokes equations and the various submodels obtained in frameworks of the asymptotic analysis sub- and supersonic flow past sharp and blunted bodies in various statements and in a wide range of numbers of Reynolds are used. Our approach is based on hierarchy of the mathematical models uniting simplicity with opportunities of complication. The choice of this or that model simplification is defined by the purposes of research. The mathematical models must be capable of capturing a variety of complex flow features such as shock waves and contact

discontinuities, vortex shedding, shock and boundary-layer interactions, flow separation and unsteady effects. Particularly, the purposes determine those physical processes that are necessary for taking into account, and what can be neglected.

The next methods were used: unsteady 3-D Euler equations solver based on method of predictor-corrector for calculations 3-D Euler with/without shock wave capturing, updating of a marching method and boundary layer approach, Navier-Stokes equations in so-called approximation of a "thin" layer, full Navier-Stokes (N-S) equations.

CFD simulations of hypersonic flows include the thermo-chemical models of the processes occurring in the shock layer the following types: chemical reactions, dissociation and recombination, exchange reactions, processes of vibration energy-exchange between various levels of molecules, influence of the vibrational relaxation on the chemical reactions (CV-processes), processes of excitation and deactivation of the electronic states of molecules. The algorithm is realized for gas-phase and gas wall interaction models of various complexities from perfect gas to multi-temperature, multi-species and thermo-chemically non-equilibrium gas medium.

Numerical methods

The computational algorithms based on numerical methods that implement a discretisation of partial differential or integral equations. There are many numerical algorithmic choices that used in deriving a solution procedure to solve mathematical physics equation. Several of these algorithms have been implemented in the finite-difference, finite-volume methods. In the the finite-difference case the derivatives changed by finite-difference analogies. For the solution of equation one can use a variety of temporal and spatial discretisations. In the second case the integration of finite volume produced by subsequent changing the volume integral on the surface integral and surface integral on linear integral with finally substitution of numerical analogies. The schemes have different accuracy order of the numerical scheme, artificial viscosity parameters in the numerical scheme, stability limit, relaxation and approximate factorization procedures. The total variation diminishing schemes, schemes with control of the "artificial" viscosity and dispersion, high order upwind schemes used. Just effective and reliable, robust numerical methods are chosen. Almost all the production level CFD codes used second-order accurate discretization of inviscid, viscous terms. Spatial discretizations used central difference to viscous terms versus upwind schemes to convective terms. Basically the schemes are explicit schemes implemented on parallel computer.

A major issue in software development is "validation." Particularly in our case we are comparing the results obtained by 4 different methods (Euler with/without shock fitting, N-S in thin layer approximation and complete N-S) for the same problem. It also involves careful examination of numerical and physical parameters used in the computations that influence accuracy, such as number of grid points, size of computational domain.

Practical methods of the geometry design

One of the basic problems at the solution of aerodynamics problems is creation of the most full computer models of geometry. The different methods of geometry designing of the complete configuration (/1, 2, 5/) will be considered. The geometry design had provided a key to the development of grid generation. The traditional techniques of generation geometry used: the spline's interpolation, algebraic methods, solid body generation. The process depends on initial information.

At the first stages it is especially important to construct the elementary model

that is taking into account the basic design parameters- *baseline approximation*. In this case it is convenient to set a surface analytically approximating by elementary surfaces. Advantage of such technique consists in that it can be used at all design levels. The analytical presentation is convenient to define a surface by finite number of parameters. The geometry is represented as set of elements of geometry (for example, a fuselage, wings etc.). Each of elements of a surface consists of set of compartments. A compartment may be expressed through geometrical parameters of section of a compartment like a wing: thickness, chord of section, curvature, etc. Let's take into account that configuration is made from separate parts and each part imposes the certain restrictions on aerodynamic characteristics. Linear and nonlinear geometrical restrictions also included in these initial objects of geometry. If the geometry is set by such manner than it is dependent on finite number of parameters with which can be easily operated. The main ideas of the abovementioned methods are implemented in the ACAD system (design system for aerodynamic purposes). This approach is useful for optimization problems.

Surface representations use the parameter cubic B-splines. Non-uniform Rational B-Spline (NURBS) support a data structure to represent all geometric primitive and have such desirable properties as local control, convex shape preserving forms, etc.

Solid body method is forming by such operations as addition, subtraction of geometry's primitives. Interactive process and visualisation algorithms are main features of this approach.

Grid generation

For last years methods of grid generation became an interdisciplinary problem. During the past two decade there has been a substantial effort to develop the rectangular, structured, unstructured grids. Specific of studied problems dictates to use the different methods for grid generation. For numerical solution of problem with complex surface geometry and complex solution structure it is necessary to use the hybrid grids combining best features of grids. Mathematical problems of grid generation are considered from point of view of the conformal mapping theory, differential geometry, theory of surfaces and tensor calculus. The main advantage of the grid is potential for an adaptation, geometric flexibility, automation.

When surface parameterization obtained then 3-D grid generation will begin. The physical region is divided into sub-regions and within each sub-region a structured grid is generated. The curvilinear grid points conform to the boundaries, surfaces, or both and therefore provide the most accurate way of specifying the boundary conditions. High quality grid can generate by the solution of partial differential grid generation methods. For solution of partial differential equations elliptic grid generator used.

One of the basic problems is the grid generation that takes into account geometrical and physical features of the flow field. The grid follows to physical meaning of solution. A mesh must highly specialize for the particular problems (resolving the different scale processes, special meshing for viscous effect, boundary layers and so on). The accuracy of computations depends on the mesh size of grid spacing in real space and the ability to control a physical mesh point's distribution. Point's concentration in the region where gradients of solution are high can help to control the accuracy. The correct adequate co-ordinate system can help to resolve the problem more easily. Boundary with node's concentration near surface demands high resolution and thin mesh. Size of mesh spacing near wall depends on Reynolds number. In our opinion just coordinate body fitted system can correctly resolved the

viscous effects.

The grid adaptation is achieved by moving the grid points and refinement. The redistribution has been the favored approach with structured grids. Thus structured grid can be adapted to the flow gradients solving the shocks, in boundary layers, etc. Thus the grid generator can be used repeatedly. A several grid technique had been developed for volume grid generation about complex 3-D configurations. Structured block's grid is formed by a network of curvilinear coordinate lines such that a one-to-one mapping can be established between the physical and computational domains.

In some cases of conformal mapping allows the sufficient preferences in solution of concrete problems. Theory of conformal mapping describes by analytical function theory of one complex variable. The conformal mapping characterised by conservation of angles. A coefficient of linear scale change does not depend on direction. It is reasonable to add that if the solution on boundary is known then it's possible to continue analytically on whole region (advance front). The conformal mapping permits to reflect an arbitrary external region on external region of unity radius circle or, another words, to design grid. Conformal mapping permits to obtain solution of new problem from known one. It is well known that the conformal mapping does not generalize to 3-D case. From point of view of structured grid generation we don't need in order to 3-D case it is fulfill all advantages of conformal mapping. We can consider a mapping that forms a subclass of the class of quasi-regular mappings.

Problems of optimization

Optimization problem includes the following sub-problems: definition of cost function; definition the major parameters subject to optimization and method of optimization. Changing of the aerodynamic shape results in changing of pressure distribution and skin friction upon surfaces and, hence, of cost function. The problem of designing may be examined as a task of management, where function of management - geometry, which gets out to optimize the function of cost subordinated to restrictions determined by the gas-dynamics and geometry.

As algorithm of optimization the descent method is used. In view of the huge expenses connected to calculation of criterion function, the deterministic methods of optimization based on gradient methods and the analysis of sensitivity, in our opinion, are more preferable. The deterministic methods of optimization are effective at a finding of minimum for which it is possible to calculate precisely the individual derivatives of design variables. As is known, if cost function and restrictions - are differentiable and convex, the optimum received by gradient methods will be a global optimum. Practically, however, it is very difficult to prove these properties. Restrictions on smoothness and necessity of derivative calculation - inconveniences in addition to that these methods find as a rule a local instead of a global optimum.

Software development and parallelization

N-S computations for complex 3-D configurations require extensive computational time on currently available computing platforms. This platform is being addressed both at the algorithm level and the computer hardware level. At the hardware level an enormous effort has been developed during past decade to parallelization of codes on massively parallel computers and clusters of workstations.

The CFD problem is solved by a decomposition domain, improving of communication between processors and with use of standards of system MPI

(message passing interface). Choice MPI as library is determined according to the requirement, that the resulting program was applicable to various parallel computing platforms to homogeneous and heterogeneous networks of the automated workplaces. At the same time the original version of the scalar codes are adapted to the parallel computer "PARAM" and a cluster. The unsteady three-dimensional problems divided among coprocessors are considered as an interconnection of unsteady two-dimensional problems interacting with each others.

A. Another problem is a parallelization of unsteady 3-D problem. In this case 3-D domain is divided on equal sub-domain in predominant (more time consuming) direction. The same code is put on different processors. Let's consider first, last, even and odd processors. Even processor receives the data from the neighbors with larger number, odd processors send the data to the neighbors with smaller number. With all necessary components determined for multi block designing, we shall allocate full procedure of calculation produce a domain decomposition; introduce a multi-block grid; divide it into the appropriate number of processors; create list of indexes for communication of cross-section cells.

Thus we can obtain solution in own sub-domain and it will communicate with neighbour's regions. For maintenance of communication between blocks of the parallel computer system the program toolkit MPI used.

B. For optimization design problem the simple way for the solution of multi-parameter problems is that for each processor the same solver are used. Therefore all details of the parallel calculations appropriate to these first two parts of the code are identical on each processor. Since algorithm of construction of geometry, on each processor the problem independently is solved at the given geometry parameters. The connections necessary for service of a sequence of geometries also should be coordinated according to the same decomposition strategy areas. For each of variables of designing we shall repeat the following procedures: to set new geometry; to construct a grid; to solve the governing equations for each block; to find the new values of aerodynamic characteristics in each block. In order to find an increment of cost function, it is necessary to solve a problem of a flow at new values of parameters of optimization. We shall calculate a direction of search with the help of a method of optimization and we shall find a direction of search.

Results

Some of the results of the CFD and CAD applications are displayed ([1-3]). The results aim to show the possibilities of mathematical models and numerical methods of flow fields modeling for incompressible, compressible and non-uniform gas. Fig.1 a,b,c,d shows the application of our ACAD system for geometries design. In Fig.2 (a,b) results of grid generation are shown. Numerical modeling flow fields past obstacles on the plane are presented (fig.3 a,b,c). Results obtained in framework of N-S equations for different Re number. The different scenarios of the separation process are realized. On fig.3c is displayed the results of streamline pattern for cavity on plane.

The calculations of flows past space vehicles were carried out on the basis of combined set of codes for computations of flows past 3-D bodies taking into account thermo-chemical non-equilibrium, shock and surface effects. The usual approach when the flow field is divided into the nose, side, base and wake regions is implemented. Different regions are then treated successively with suitable techniques. Calculations of the convective heat flux were carried out for along the forebody of a vehicle entering in the Martian atmosphere and having the form of 120 degree spherically blunted cone ($R=1m$, fig.4a, b). There the free-stream conditions are set as follows: $H=40-60$ km, $V_{\infty}=3.5-6.0$ km/s, $T_w=1500^{\circ}K$, $Re=3-5.10(5)$ -and "s" is a distribution along body

length (fig.5). Different vibrational energy transitions between and within three vibrational modes were taken into account. The computation of the forward section of geometry within the framework of Navier-Stokes and non-equilibrium gas is shown in Fig.5a,b. Calculations were performed for three approaches: thermal equilibrium-1, two-temperature-2 and three-temperature thermal non-equilibrium approaches -3. Heat flux distributions q_w is shown along body length. These results are shown for two cases: catalytic(5a) and non-catalytic surface(5b).

Acknowledgements

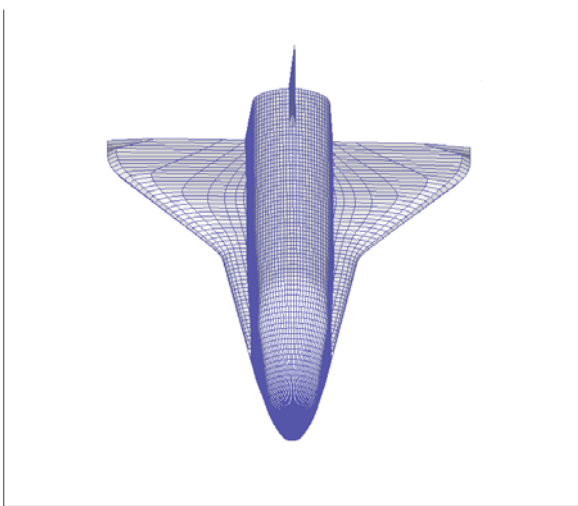
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The conclusion

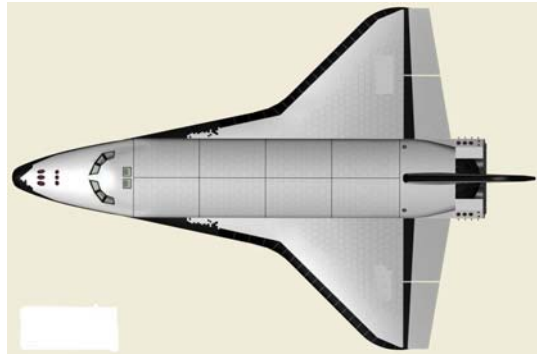
For the solution of real technical problems the new generation of the software which will allow solve questions of the automated design is required; to automatically grid generation, to take into account main features of complex domain topology, to use of new numerical methods, transfers and process of the information, to develop of platforms with elements of an artificial intellect. Perspective directions of activity are examined.

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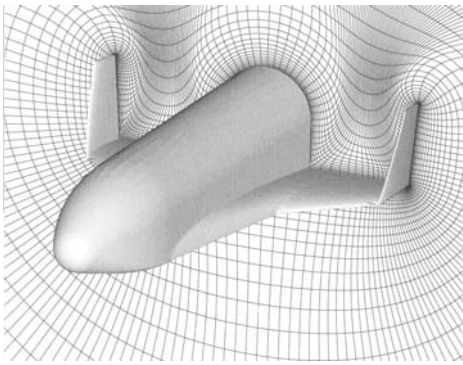
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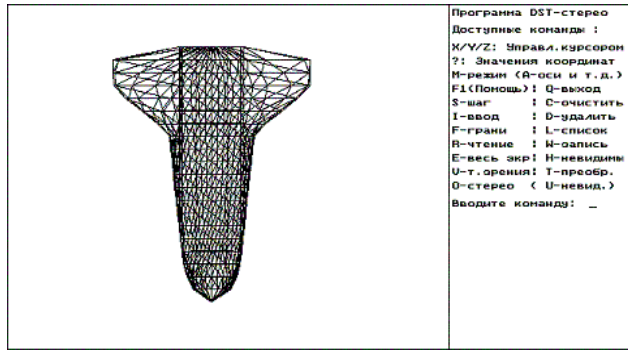
a)



b)



c)



d)

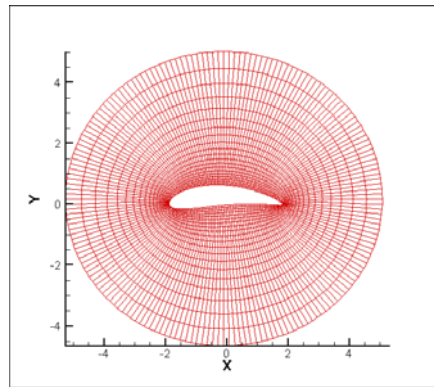
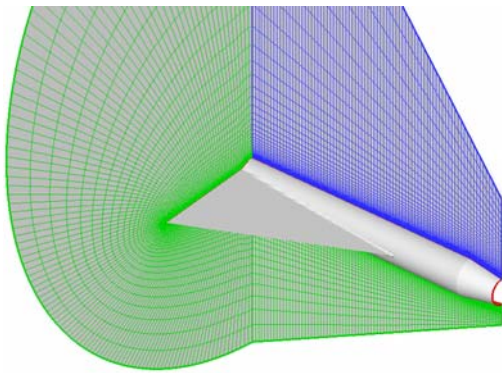


Fig.2 a,b
d)

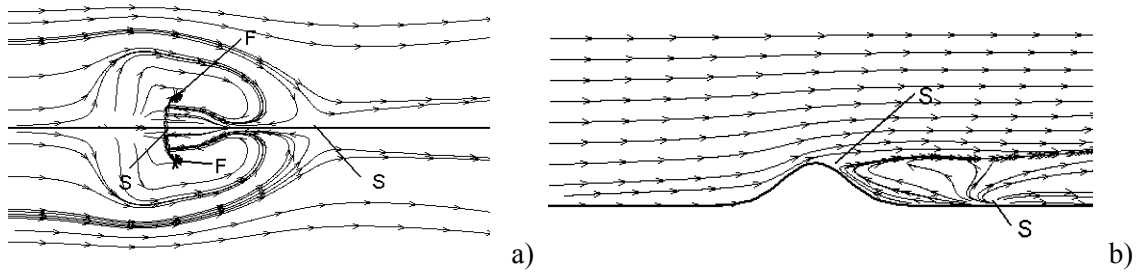


fig.3 a,b,c

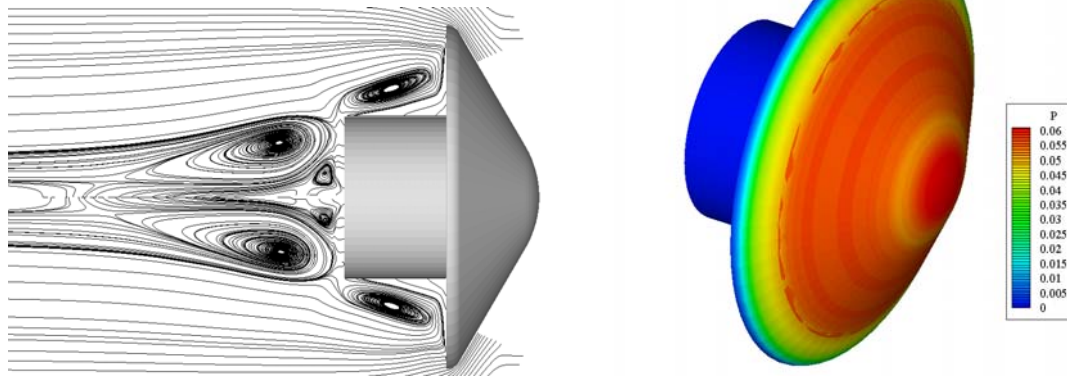
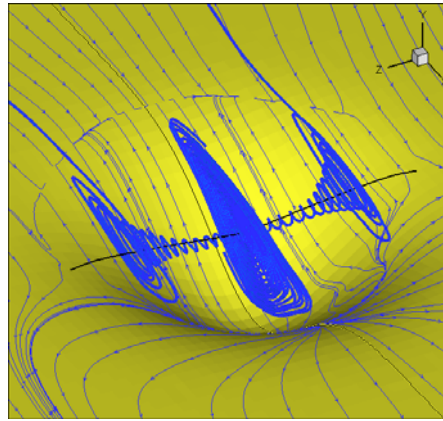
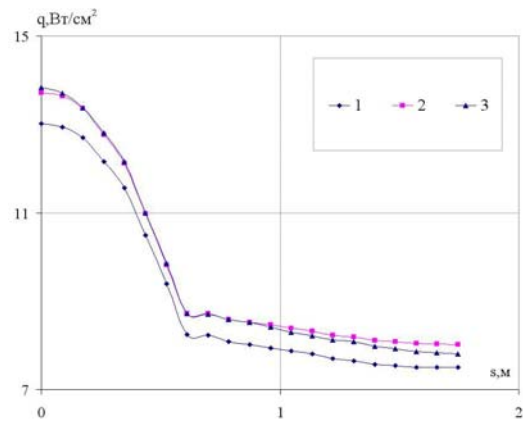
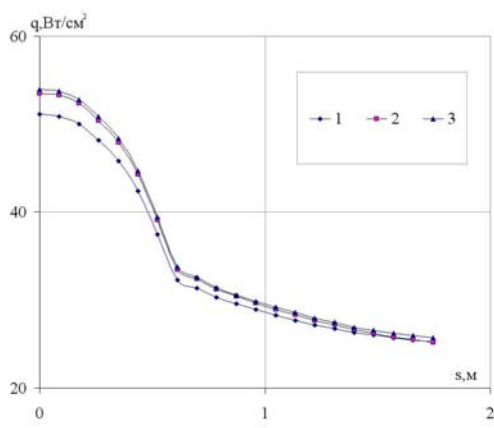


fig.4 a,b



a)
fig.5a,b

b)