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Analysis of Space-Time Structures Appearance for Non-Stationary CFD Problems

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Abstract

The paper presents a combined approach to finding conditions for space-time structures appearance in non-stationary flows for CFD (computational fluid dynamics) problems. We consider different types of space-time structures, for instance, such as boundary layer separation, vortex zone appearance, appearance of oscillating regimes, transfer from Mach reflection to regular one for shock waves, etc. The approach combines numerical solutions of inverse problems and parametric studies. Parallel numerical solutions are implemented. This approach is intended for fast approximate estimation for dependence of unsteady flow structures on characteristic parameters (or determining parameters) in a certain class of problems. The numerical results are presented in a form of multidimensional data volumes. To find out hidden dependencies in the volumes some multidimensional data processing and visualizing methods should be applied. The approach is organized in a pipeline fashion. For certain classes of problems the approach allows obtaining the sought-for dependence in a quasi-analytical form. The proposed approach can be considered to provide some kind of generalized numerical experiment environment. Examples of its application to a series of practical problems are given. The approach can be applied to CFD problems with ambiguities.

Keywords: space-time structures, parallel computations, multidimensional data

1 Introduction

The main factor defining current state in mathematical modeling is intensive development of high-performance computing and parallel algorithms. This is especially important for CFD problems because application of parallel computations allows to transfer CFD mathematical modeling to a new level. Being applied to direct CFD problems parallel computing enables to speed up the computations to use finer resolution grids in numerical experiments. Naturally, it makes the numerical experiments for standard direct problems very effective, especially for modeling of time-dependent processes. Time-dependent processes are important in computational fluid dynamics (CFD) studies. These processes are often accompanied by appearing of changeable space-time structures in the flow, such as

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separation zones, circulating flows, vortex bursts, etc. The presence of such time-dependent structures in the flow cause many undesirable effects in practice: reduced lift, airframe and control vibrations, audible noise. Space-time structures can appear and disappear in the flows defining the flow pattern and quantitative characteristics of the flow field. Simulating these changeable structures is therefore an important aspect of CFD.

The proposed new approach in mathematical modeling is an opportunity to solve multidisciplinary problems, inverse problems and parametric studies. As it is known these three types of problems are high-priority problems for modern parallel computing. Multidisciplinary problems provide combination of models for different physical processes in one numerical experiment.

Inverse problems are problems where causes for a desired or an observed effect are to be determined. The causes are unknown so one should determine them based on observation of their effects. This is in contrast to the corresponding direct problem, whose solution involves finding effects based on a complete description of their causes. The inverse problems are very important or practical engineering, where the typical problem is the choice of desired variant from the set of admissible ones. This can be the choice of a geometric shape, the choice of flow control, etc. The inverse problems are classified as boundary searches, coefficient searches, and retrospective inverse problems (Beck J.V., Blackwell B., St.Clair C., 1985).

Parametric studies allow to get numerical solution not for particular CFD problem only, but for the whole class of problems. For such cases the class of problems is defined in multidimensional space created by characteristic (or determining) parameters of the problem under consideration. These characteristic parameters are varying in definite ranges. Parametric studies are very difficult and require a lot of computer resources. But the procedure of parameter optimization and analysis is the most difficult numerical research. It is a kind of standard parametric studies where the inverse problem is considered for each point of grid in multidimensional space of characteristic parameters instead of direct problem. This type of numerical research is intended for finding the domains in the space of determining parameters where a phenomenon of interest occurs for a certain class of problems.

Such types of numerical research have one specific feature from the point of view of visualization. Their numerical results are presented in general discrete form as multidimensional arrays for grid points set in the space of characteristic parameters. The dimensionality of such array corresponds to the quantity of determining parameters. The arrays need processing and visual presentation for analyzing and comprehension. Visualization methods are applied to such array with purpose to bring out hidden dependencies.

To bring out hidden dependencies one should combine visualization approaches with Data Analysis methods for decreasing of dimensionality (Bondarev A.E., Galaktionov V.A., 2013). It is necessary due to the evident lack of visualization concepts and tools for spaces having more than 3 dimensions.

2 Problem statement

The procedure of parameter optimization and analysis requires multiple inverse problems solution. For parameter optimization and analysis one should find the determining parameters where a phenomenon of interest occurs in a certain class of problems, defined by characteristic parameters varying in definite ranges. In general, the problem statement for this procedure can be presented in accordance with (Bondarev A.E., Galaktionov V.A., 2013) as follows.

Let's suppose we have some mathematical model describing time-dependent CFD process and reliable numerical method for simulation. So we are able to simulate the direct problem for this process. During the simulation some event occurs inside the flowfield. For the problem under consideration a numerical solution $F=F(x, x_1, \ldots, x_n)$ is formed as a result of simulation. This solution is defined by control parameter x and finite set of characteristic (determining) parameters $(x_1, \ldots, x_n)$.

Let X denote $X=(x, x_1,..., x_n)$.

Then we can consider *event functional* $J(F(X))$. Just as logical variable so the functional has two values:

$J(F(X)) = 1$ – If the event of interest occurs (independently on the event details),

$J(F(X)) = 0$ - if the event of interest doesn't occur.

Let x' denote the value of control parameter when the considered event appears. Thus, the problem is to find the value x' with suitable accuracy.

As a result we obtain the sought-for value $x'(x_1^*,..., x_n^*)$ of control parameter for fixed set of determining parameters $(x_1^*,..., x_n^*)$. But the whole problem is constructing of dependence $x'(x_1,..., x_n)$ for all possible sets of determining parameters inside the ranges under consideration.

If we have a grid containing, for instance, M grid points for each characteristic parameter, then we should solve M^n similar inverse problems with purpose of finding the values x' for all grid points $(x_1^*,...,x_n^*)$ in the space of characteristic parameters. After solving M^n inverse problems one obtains all grid points where event in hand occurs in the space of characteristic parameters.

Considering the determining parameters $(x_1,...,x_n)$ as a set of basis vectors, one can present the space of the determining parameters $L(x_1,...,x_n)$ having n dimensions.

Then for general case the inverse problem can be formulated as the problem of finding in this space L all the subdomains L^* where the event of interest is observed, i.e. $J(L^*) = 1$.

At the same time the problem of data filtration is solved. Setting the ranges for characteristic parameters one can not guarantee the fact of appearance of the sought-for event inside the range. So if the event in question is not observed for some point of space $(x_1,..., x_n)$ at all (i.e. for all values of control parameter x), this point is not considered.

Such approach can be quite useful if we are dealing with CFD problems having ambiguity in solution. There are some well-known CFD problems with dual type of solution such as Mach and regular reflection for shock waves or oscillating and non-oscillating regimes for flow interacting with solid surface, etc. All these processes are expressed by changing of existing time-space structures. Using the proposed approach one can trace the transfer from one type of solution to another one in multidimensional space of characteristic parameters.

In the final analysis such general problem statement allows to get the conditions of unsteady event appearance not for separate problem only, but for the whole class of problems. The class of problems is determined by the set of characteristic parameters varying in definite ranges.

It is necessary to note that for common case we have not any theoretical criterion of selecting a control parameter from the set of characteristic parameters. For each specific class of CFD problems the main criterion of control parameter choice is practical experience basing on previous numerical and physical experiments.

3 Parallelization

The whole algorithm for parameter optimization and analysis (POA) requires to solve very large number of inverse problems (M^n, if we assume M^n grid points for each from n directions). Each of these inverse problems assumes solving of many direct problems. It makes the whole procedure of computation laborious, especially for large and complex flows. The only way out of this situation is applying of parallel computations. The problem of the optimal and effective way of parallelization was thoroughly discussed in the paper (Bondarev A.E., Galaktionov V.A., 2013). There were considered parts of the whole algorithm for parameter optimization and analysis. For these parts the main criterion of applicability for parallelizing is independence of specific numerical method. From this point of view the most perspective way for parallelizing is applying the approach of *multitask parallelism* using the principle "one task – one process". Due to minimal quantity of internal exchanges between the processes we are able to create an effective practical tool for POA.

The general parallel computing scheme used for parameters analysis and optimizing is shown in Figure 1.

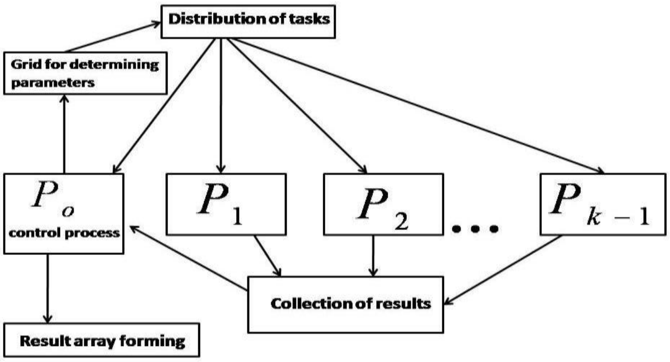

Figure 1: Parallel computing scheme for POA.

We assume that k processes are provided for parallel computation. The control process P_0 creates the grid in the multidimensional space of determining parameters, then P_0 forms tasks and sends the tasks to others processes and to itself also. After task completion P_0 collects the results and implements all procedures defined by user, such as data processing and transformation.

Due to the absence of internal exchanges between the processes the procedure of parallelizing amounts to creation of control interface for tasks distribution and data collecting in one multidimensional array.

There are two effective and easy ways to create such interface for parallel computations. The first way is to apply MPI (Message Passing Interface) (Pacheco, 1997). This variant of parallelizing allows implementing a program tool for POA. The computation can be carried out k times faster according to the number of provided processes.

The other way of parallelization is application of DVM technology (DVM-System, 2015), elaborated in Keldysh Institute of Applied Mathematics RAS. DVM-system provides unified toolkit to develop parallel programs of scientific-technical calculations in C and Fortran. DVM parallel model is based on data parallel model. The DVM name reflects two names of the model - Distributed Virtual Memory and Distributed Virtual Machine. These two names show that DVM model is adopted both for shared memory systems and for distributed memory systems. DVM high level model allows not only to decrease cost of parallel program development but provides unified formalized base for supporting Run-Time System, debugging, performance analyzing and prediction. Unified parallel model is built in C and Fortran languages on the base of the constructions, that are "transparent" for standard compilers, that allows to have single version of the program for sequential and parallel execution. C-DVM and Fortran DVM compilers translate DVM-program in C or Fortran program correspondingly, including parallel execution Run-Time Support system calls. So only requirement to a parallel system is availability of C and Fortran compilers. This way of code parallelizing allows one to save a lot of human resources for coding and debugging. At the same time DVM parallelization provides less speed of computations in comparison with MPI.

For both types of parallel technologies control interfaces for parameter optimization and analysis were designed. Both control interfaces were applied to jet interaction problem for testing. Testing computations were carried out for 20 processors. According to test results the time of computations for

DVM method is 205 seconds. The same test for MPI case requires 144 seconds. At the same time DVM application allowed to decrease human expenses for coding and debugging up to ten times as against MPI. So both types of parallel technologies are quite applicable for problems in question.

As a result of such computations one obtains control parameter dependence on determining parameters in general discrete form as n-dimensional array $x'(x_1,\dots, x_n)$.

4 Multidimensional Data Analysis

For practical CFD problems the main goal of simulation is usually obtaining the control parameter dependence on determining parameters of the problem in quasi-analytical form or in tabulated form. As a matter of fact obtaining such dependencies have been the main point of practical CFD applications last 50 years.

Using described above approach for parameter optimization and analysis one obtains control parameter dependence on determining parameters in general discrete form as n-dimensional array $x'(x_1^*,\dots, x_n^*)$ for grid points in the space of characteristic parameters.

It is necessary to note that multidimensional data analysis was not used in CFD problems before last years. The methods and approaches of *Scientific Visualization* (Bondarev A.E., Galaktionov V.A., Chechetkin V.M., 2011) were quite sufficient for analyzing even the most complicated CFD processes. But at the current time we are able to solve the problems of POA and parametric studies. The solutions of such problems are multidimensional data volume, so one should be able to process and analyze the data with final purpose to find out the sought-for dependencies.

The form of multidimensional array is not suitable for practical analysis. The most effective way of finding the sought-for dependence in a quasi-analytical form is a visual presentation of array.

If we have visual presentation of data array, we are able to approximate the data (where it is possible) by simple geometric elements, such as lines, planes, parts of spheres etc. After approximation we can present the sought-for dependence as a quasi-analytical expression.

Due to evident lack of adequate visual concepts for data volumes with dimensionality number more than three (Bondarev A.E., Galaktionov V.A., Chechetkin V.M., 2011) one should try to decrease the volume dimensionality up to 3 with purpose to apply standard *Scientific Visualization* methods after decreasing.

There are some ways to decrease the array dimensionality. These ways are well known from the group of methods for multidimensional data processing and analysis. Being frank we should note the fact that most of these methods were used for a long time before computers appearance. This field of science was known as “experimental data processing”.

The first way is the analysis of variances for each characteristic parameter. Characteristic parameter is considered as coordinate direction. Data variances $D_1, D_2, \dots D_n$ are computed along the each direction. Then the variances should be arranged. The direction with minimal variance $D_{min} = \min\{D_i\}$ is rejected. This procedure sometimes is called as compactification.

More radical kind of compactification can be implemented as follows. After variances computing and arranging one chooses three directions with maximal variances. If other variances are much less than this triplet one changes the data for directions corresponding to other variances by means. After such decreasing of dimensionality one can operate in standard 3D space. This approach has one disadvantage - it does not work if multidimensional data are close to hypersphere. Nevertheless for many practical cases with small dimensionality (4 or 5) the approach works well enough.

Another way is the construction of different 3D data projections for various triplets of determining parameters. If the data on projections for some direction are close to constant then this direction can be rejected.

Both approaches are not based on any scientific theory. The approaches are the ways of creation some hypothesis about data in question. But both approaches allow to obtain real results in practice.

Applying *Data Analysis* methods one can use PCA method (Principal Component Analysis) with purpose to decrease the number of dimensions (Zinovyev, 2000). The principal component is a direction in multidimensional space with maximal data variance along. PCA method application is based on localization of 3 principal components and data presentation using these components as new coordinate system. So this method provides the choice of a new orthogonal basis with coordinate directions corresponding to the variances arranged in descending order. For the case of data with complex topology PCA method is generalized. The generalized method is called principal manifolds method (or principal curves) (Gorban A., Kegl B., Wunsch D., Zinovyev A. (Eds.), 2007).

PCA method allows one to project original array to plane or to 3D space created by principal components. Before PCA applying one should make a decision how many principal components are required for adequate description of multidimensional data volume under consideration. For this purpose one should compute and arrange eigenvalues for covariance matrix built from original data. The best variant is that one where 2 or 3 principal components provide the main income to general variance of data volume.

For this case the scheme of data volume processing looks as follows.

For original data volume we define 3 first principal components Y_1, Y_2, Y_3 , where each of them is a linear combination created from original variables $Y(x_1, \ldots,x_n) = \sum B_i x_i$. Then the points from original data volume are transferred to principal components

$A_i(x_1, \ldots,x_n)= A_i(Y_1(x_1, \ldots,x_n), Y_2(x_1, \ldots,x_n), Y_3(x_1, \ldots,x_n))$.

Then one can easily implement 2D visual presentation $A_i(Y_1,Y_2)$ or 3D one $A_i(Y_1, Y_2, Y_3)$. The visualization allows one to estimate the shape of dependencies in the data volume and to approximate the shape by geometric primitives having analytical form. For the simplest case one can apply rough linear approximation by parametric plane. Using inverse transformation for the approximating parametric plane one obtain the sought-for quasi-analytical dependence in original variables. If using of one approximating parametric plane is insufficient then one can use a set of such planes.

Combining these methods we can decrease the array dimensionality for many practical cases.

5 Applications

This section contains the examples of the proposed above approach applied to some practical problems. It is applied in some variations due to different aims for each class of problems.

The first example is the problem of unsteady interaction of the supersonic viscous flow with jet obstacle (Bondarev, 2014). Figure 2 illustrates the example. The obstacle appears due to co-current underexpanded jet exhausting from the nozzle. The nozzle is placed to external supersonic viscous flow. Expanding jet propagates on the external surface of the nozzle creating obstacle in external flowfield. Typical flow structure is shown in Figure 2 (a) by streamlines. Time-dependent control action (the velocity of pressure ratio growth in underexpanded jet) allows to change time-space structure of flowfield (Figure 2 (b)). New space-time structure presents specific flow regime where jet propagates upwind on the external wall of the nozzle. We consider crucial velocity of jet pressure ratio growth as control parameter. The main target of research is estimating and defining the control parameter dependence on four characteristic parameters of the problem – Mach, Reynolds, Prandtl and Strouhal numbers. These parameters are varied in definite ranges creating four-dimensional space. We want to find for each point in this space the crucial velocity corresponding to a new time-space structure appearance.

According to the scheme presented in the previous chapters parallel algorithm is implemented for computations. For the space of determining parameters two types of grids are chosen: 5 and 10 points for each determining parameter. It requires computing 625 and 10000 inverse problems. The computations are performed by parallel cluster K100 (Keldysh Institute of Applied Mathematics RAS, Moscow, Russia). Both MPI and DVM technologies were applied to control parallel computations.

As a result of approach application five-dimensional data array is obtained, where variables are four characteristic parameters M_∞, Re_∞, Pr, Sh_∞ and crucial velocity V^*. For obtained data three principal components are defined and we construct data visual presentation in principal components (Figure 2 (c)). The presentation allows us to suppose that the points of data volume can be roughly approximated by parametric plane. After defining the coefficients for plane and inverse transformation to the original variables we obtain the sought-for dependence $V^* = F(M_\infty, Re_\infty, Pr, Sh_\infty)$ in analytical form. Obtained results present a solution of parameter optimization and analysis for the class of problems, where the class is defined by multidimensional volume of characteristic parameters.

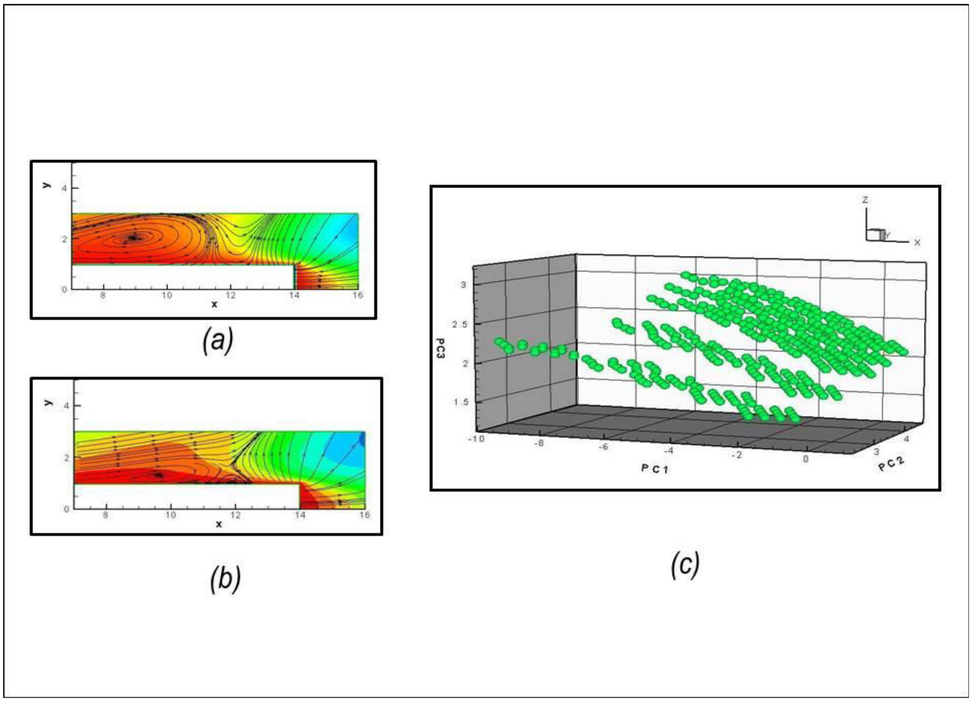

Figure 2: Parameter optimization and analysis applied to jets interaction

Another example of approach application is quite close to previous one. We consider time-dependent processes of supersonic underexpanded jet interaction with flat plate (Alexeev A., Bondarev A., 2014). Numerical investigations are performed to study some special modes of interaction. The goal of studies is to consider the conditions for existence of oscillating mode where separation zones can appear and disappear. Figure 3 (a) presents the flowfield by density distribution for the problem in question. The separation zones appear in the vicinity of the point where the jet meets flat pate. The presence of oscillating mode is illustrated by pressure on the symmetry axis in dependence on time Figure 3 (b).

Underexpanded supersonic jet propagates up to flat plate. For some conditions vortex zone can appear in the vicinity of flat plate. This zone begins to appear and disappear in oscillating mode. The target of research is to define the conditions of oscillations appearance. There are some known experimental results for this class of problem (Glaznev V., Zapryagaev V., Uskov V. , 2000). So we know in advance that for this problem we have three characteristic parameters – Mach number M_∞, jet pressure ratio *n*, specific heat ratio *ɣ*. The distance from jet to plate *x* is considered as control parameter. According to (Glaznev V., Zapryagaev V., Uskov V. , 2000) the control parameter dependence on characteristic parameters can be presented by expression $x^2 \sim 16\ \gamma\ n\ M_\infty$. This dependence is a condition for oscillating mode appearance. The computations confirm this experimental fact.

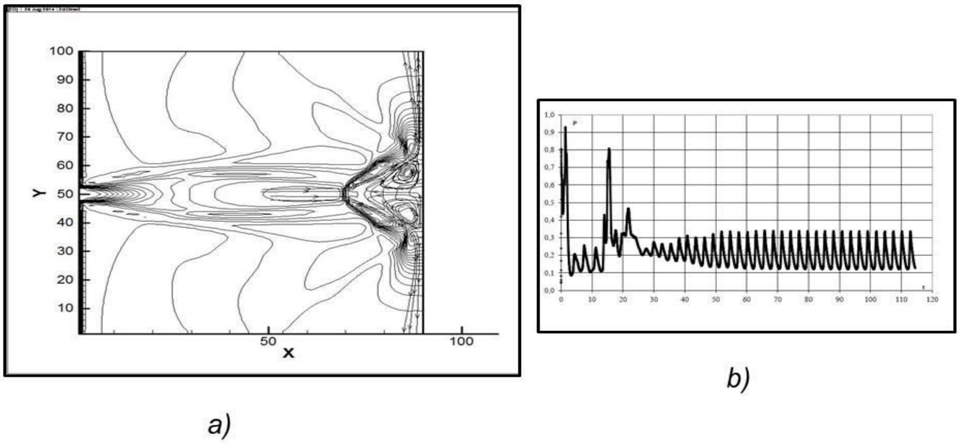

Figure 3: The search of oscillating regime appearance in jets interacting with plate.

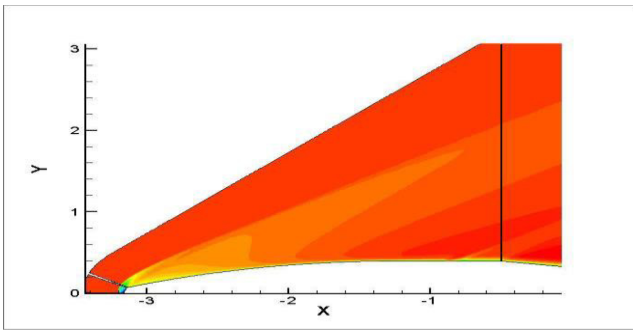

Figure 4: Axisymmetric body in the supersonic flow.

The next example of approach application can be referred to parametric studies. We consider time-dependent gasdynamic processes around axisymmetric body placed in the supersonic flow (Figure 4). The problem is to define aerodynamic coefficients for the body in dependence on time, velocity, viscosity, humidity, height of the flight, angle of attack. To compute the dependence we should use parallel computations according the approach described in previous sections. As a result we obtain multidimensional data array. To process the data in array we apply described combined approach including analysis of variances and principal components. As data processing result we obtain aerodynamic coefficients dependencies on characteristic parameters by approximation. The results of approximation can be used further for computations of flight parameters.

The examples show applicability of presented approach for a wide range of practical applications, so the approach can be considered as quite universal one.

6 Discussion

Described in previous sections methods and approaches are intended to be integrated in a whole set. This set is built as technological chain of algorithms or pipeline for multidimensional data producing, processing and analyzing. Such chain one can consider as some kind of prototype of generalized experiment for fluid dynamics problems. The scheme for implementation of such generalized experiment is presented in Figure 5.

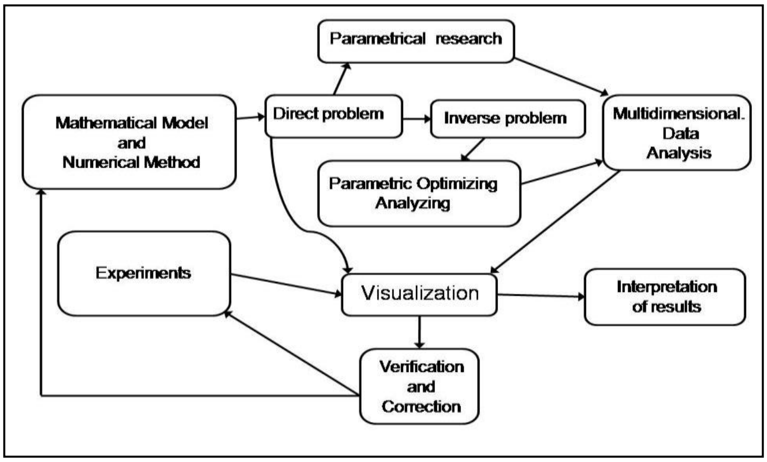

Figure 5: Scheme of generalized experiment.

This experiment is to be based on reliable mathematical model, numerical method and capabilities of experimental research. The methods for searching and tracing of time-dependent structures in the flow under consideration should be integrated in the set of methods. Such generalized experiment should be able to solve inverse problems and optimization problems. During the process of numerical computation the results are to be directly compared with experimental ones for all possible cases. It would provide the process of constant verification. Being implemented by means of parallel methods the properties mentioned above would provide a possibility of parametric studies and parameter optimization and analysis. These approaches would give us the results in a form of multidimensional arrays. To analyze the results one should use Data Analysis methods, which should be integrated in the set of numerical methods for generalized experiment. Finally the future generalized experiment would provide solution for classes of CFD problems. It can be very effective for practical applications. Constant verification is to be used for improving of numerical methods and conditions of experiment.

Such generalized numerical experiment is quite universal. It can be applied to many time-dependent processes in mathematical modeling. The implementation of such generalized numerical experiment should provide large-scale computations for industrial purposes.

7 Conclusions

The paper considers combined approach to finding of conditions for space-time structures appearance in non-stationary flows for CFD problems. The approach allows to estimate how the crucial points of flow structure transformation depend on determining parameters of the problem. Considered problem of parameter optimization and analysis amounts to solving a set of similar small tasks, so it can be applied also for parallel computations. The results of such computations are multidimensional data volumes. The main purpose is to find hidden dependencies in such volumes. For some practical cases one can apply Data Analysis methods for decreasing number of dimensions up to three. Then one can approximate the resulting dependence by geometric primitives. The approximation allows to obtain the sought-for dependencies in a quasi-analytical form. The approach can be applied to studies of CFD problems with ambiguity to determine the domains for different branches of solution in multidimensional space of characteristic parameters.

Being organized for data producing, processing and analyzing in a form of pipeline the approach can be considered as a prototype of generalized numerical experiment.

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References

Alexeev A., Bondarev A. (2014). Mesh methods for boundary-value problems and applications. Proceedings of 10th International Conference. *Modeling of Time-Dependent Modes for Supersonic Underexpanded Jet Interacting with Plate* (pp. 64-68). Kazan: Otechestvo.

Beck J.V., Blackwell B., St.Clair C. (1985). *Inverse Heat Conduction. Ill-posed Problems.* NY: John Wiley&Sons.

Bondarev A.E., Galaktionov V.A. (2013). Parametric Optimizing Analysis of Unsteady Structures and Visualization of Multidimensional Data. *International Journal of Modeling, Simulation and Scientific Computing, 4*(suppl. issue 1).

Bondarev A.E., Galaktionov V.A., Chechetkin V.M. (2011). Analysis of the development concepts and methods of visual data representation in computational physics. *Computational Mathematics and Mathematical Physics, 51*(4), 624-636.

Bondarev, A. (2014). Multidimensional Data Analysis in CFD Problems. *Scientific Visualization, 6*(5), 61-68.

DVM-System. (2015). Retrieved January 2015, from http://www.keldysh.ru/dvm/dvmhtm1107/eng/dvmINTRe.htm

Glaznev V., Zapryagaev V., Uskov V. . (2000). *Jets and unsteady flows in gas dynamics [Struynye i nestacionarnye techeniya v gazovoy dinamike]*. Novosibirsk: SB RAS.

Gorban A., Kegl B., Wunsch D., Zinovyev A. (Eds.). (2007). *Principal Manifolds for Data Visualisation and Dimension Reduction* (LNCSE 58 ed.). Berlin – Heidelberg – New York: Springer.

Lee K., Hong S. (2004). Supersonic Jet Impingement Navier-Stokes Computations for Vertical Launching System Design Applications. *J. SPACECRAFT&ROCKETS, 41*(5).

Pacheco, P. (1997). *Programming Parallel with MPI.* San Francisco, CA: Morgan Kaufmann.

Zinovyev, A. (2000). *Vizualization of multidimensional data [Visualizaciya mnogomernyh dannyh]*. Krasnoyarsk: Krasnoyarsk Univ.