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MULTIBLOCK PARALLEL COMPUTATION OF AN INCOMPRESSIBLE 3-D FLOW IN TURBOMACHINES

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Abstract: A finite volume numerical method for the prediction of a fluid flow in complex geometries, such as turbomachinery channels, has been parallelized using a domain decomposition approach. A mathematical formulation of a 3-D incompressible steady flow has been presented on the basis of the N-S equations in a grid-oriented co-ordinate system with contravariant velocity components. A parallelized pressure-based implicit algorithm with discretization on a staggered grid has been developed. A message exchange system with a boundary exchange, developed by the authors, has been described. Exemplary calculations have been carried out for a laminar flow through a curved duct and for an inviscid flow through a stage of the centrifugal pump. A good agreement has been obtained in both cases. Despite considerable simplification that has been introduced in the flow through the pump stage, the computations have shown nearly the same pressure rise in the stage as the measurements. Further directions of numerical investigations of a flow through turbomachines, including in particular those devoted to pressure losses related to the rotor-stator interaction, have been mentioned.

Keywords: numerical simulations, turbomachinery, incompressible flow, 3-D Navier-Stokes solver, parallel computing

1. Introduction

Internal flows through turbomachinery channels belong to the most complicated cases the fluid dynamics is interested in. The numerical research in these cases has become competitive with the experimental one. However, numerical and experimental methods used together bring outcomes consisting of more information than a simple sum of them. Furthermore, they test each other and are complementary to each other. A combination of them seems to be the best way of engineering investigations of the flow phenomena.

The complexity of the turbomachinery flows in their numerical simulation is caused by a complicated character of the flow phenomena and by treatment of a generic diversity of the walls of channels and their mutual location of them. The first group of issues is essential and refers to the uncertainties of the models of physical effects, such as turbulence or unsteady components of the flow associated

with the rotor-stator interaction. Surmounting these issues is still connected with an art of introducing proper simplification. To overcome the problems of the complex geometry, a grid based on a curvilinear, non-orthogonal co-ordinate system has been used in this paper rather than grids which are defined without any relation to a co-ordinate system. Also a domain decomposition can be applied to cover a wall shape diversity, as well as a complexity of the channel arrangement of the flow system. The next reason for employing the domain decomposition is that parallel computation can easily be carried out on the decomposed domain.

Determination of a 3-D fluid flow by means of computational fluid dynamics methods has become a useful engineering tool for investigation and design of turbomachines. A need to solve complex tasks in acceptable time leads to the problem of increasing the computing speed. A need to undertake investigations on fast algorithms is placed on the first position of Lakshminarayan's recommendations [1] for further development of CFD applications in analysis and design of turbomachines, whereas on position no. 7 of his recommendations he gives one possible way to obtain it - to adapt codes for massive parallel computers. The present state of development of hardware, availability of multiprocessor computers with shared memory, fast networks of work stations, make parallelization of computations necessary in order to use the hardware effectively and to reduce the time needed to solve a task.

There are two possible approaches towards CFD task parallelization: task functional decomposition and domain decomposition. The latter one consists in decomposition of the task domain into subdomains and assigning one processor to each subdomain. The communication among them is needed to exchange data and to synchronize computations. Parallelization of CFD schemes with the domain decomposition is used to accelerate linear solvers dealing with internal iterations, Seidl et al. [2], or to accelerate the global iterative procedure, as in Schieweck [3].

Apart from accelerating solvers, in the case of application for turbomachines, the domain decomposition can be introduced independently whether parallelization

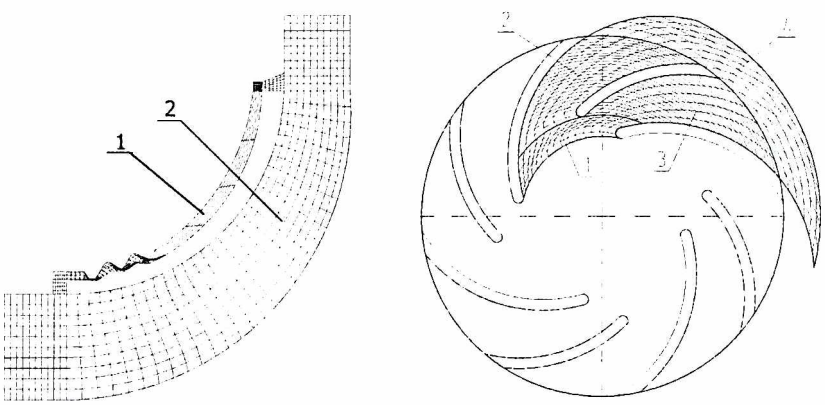

Figure 1. *Sample schemes of the domain decomposition, 1, 2, 3, 4 — computational subdomains.*

exists or not. It is forced by the complexity of shapes of channels and their reciprocal arrangement. This kind of reasons for the domain decomposition occurs in a flow simulation through a full stage of the centrifugal pump. Sample schemes of the domain decomposition, dependent on the task concerning the flow in a turbomachine, are presented in Figure 1.

2. Governing Equations and Solution Method

The code for simulation of internal viscous compressible and incompressible flows has been written in Fortran 77 on the basis of an algorithm belonging to the SIMPLE group (Palankar [4]). The governing equations are formulated in the boundary fitted co-ordinates that are mapped numerically on a Cartesian or cylindrical co-ordinate system by means of the grid. The equations of mass and momentum conservation for a steady flow in the invariant formulation with the contravariant velocity components have the following form:

$$\frac{\partial}{\partial x^j}\left(\frac{\rho v^j}{\Im}\right)=0,$$

$$N^n[\rho,v]-\frac{g^{nk}}{\Im}\frac{\partial p}{\partial x^k}=0;\quad n=1,2,3,$$

where the differential operator N^n is:

$$N^n[\rho,v]\equiv\frac{\partial}{\partial x^j}\left(-\frac{\rho v^j v^n}{\Im}+\frac{\tau^{nj}}{\Im}\right)+\frac{1}{\Im}\Gamma^n_{ij}\left(-\rho v^i v^j+\tau^{ij}\right)+\frac{\rho f^n}{\Im},$$

and the centrifugal and Coriolis forces f^n are given with the notation of tensor analysis [5]:

$$f^n=|\omega|^2 r^n+2\varepsilon^{njk}\omega_j v_k\Im.$$

On the basis of the concept of the effective viscosity, the shear stress tensor is expressed as:

$$\tau^{nj}=\mu_e\left(g^{jk}\frac{\partial v}{\partial x^k}+g^{nk}\frac{\partial v}{\partial x^k}-\frac{\partial g^{nj}}{\partial x^k}v^k\right)$$

or can be assumed to be equal to zero for an inviscid flow.

The boundary fitted curvilinear coordinate system denoted as (x^1, x^2, x^3) has metric properties described by the metric tensor g^{nk}, the Christoffel's symbol Γ^n_{ij} and the Jacobian $\Im$.

The N-S equations applied to a flow through turbomachinery channels are characterized by the fact that the convection terms dominate over the diffusion ones. Therefore, the boundary conditions suitable for the Euler equation have a strong influence, other boundary conditions are posed on the diffusive terms and have a weak effect on the solution.

The boundary conditions have been assumed on the channel wall surfaces (the velocity vanishes), the periodicity surfaces supplemented by inlet and outlet surfaces. The value of pressure is determined on the outlet surfaces, whereas 3 algebraic equations, solvable with respect to 3 velocity components, are posed on the inlet surfaces. For a diffusion term, 2 additional equations are required for each outlet surface to couple the components of the stress tensor and 2 tangent velocity components at the outlet. They are weak boundary conditions.

The discretization has been carried out with the finite volume method with staggered grids aligned to the curvilinear co-ordinate system. The equations have been discretized by means of the second order central schemes, except for the convection terms, for which the first and second order upwind approximation has been introduced. In the calculations presented in this paper only the first order upwind scheme has been used. The pressure correction method has been employed to solve the system of algebraic equations which resulted from the discretization of the governing equations. The algorithm is discussed in detail in [6] and [7].

3. Domain Decomposition

The parallelization has been carried out by means of a domain decomposition into non-overlapping subdomains in space — the so called multiblock decomposition. Two different multiblock approaches are used to link the equations on the neighboring blocks.

The first one, used for non-overlapping blocks only, is reduced to the arrangement of the iterative procedure in which the sweeping is carried out on the neighboring blocks [8]. The process can be sequential or parallel. Apart from its own nodes and cells, each block includes an overlapping area composed of one or several layers of nodes and cells imposed on the neighboring blocks. The memory region corresponding to the overlapping area is updated by means of a suitable algorithm to comply with current values of variables being iterated on the neighboring block.

According to the second approach, computations are carried out on each block providing data to pose the boundary conditions on the neighboring blocks. This way of treating subdomains is generally used in the Schwartz's method, in which blocks overlap. In the present paper this second approach has been used but blocks do not overlap. The advantage of this approach lies in the fact that it can be adapted to grids which do not match at interfaces and which are subject to an overlapping decomposition.

The discretization of governing equations has been carried out in each subdomain on a regular structural grid with a local curvilinear co-ordinate system on gridlines fitted on each domain separately. Grids have to match at their interfaces to share common nodes, gridlines and cell faces. These grids are called block-structured grids which match at interfaces. A sample 2-D grid of this kind consisting of 3 blocks has been presented in Figure 2. Although the grids in subdomains and in the places they overlap exhibit a curvilinear character in order to

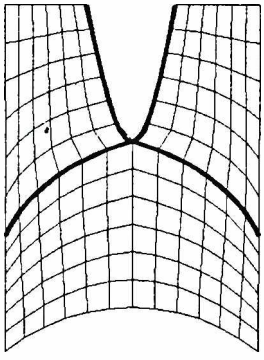

Figure 2. *Example of the 2-D block-structured grid which matches at interfaces.*

adapt to the wall shape, from the topological viewpoint (after straightening) they have a character of a cuboid. A decomposition of the whole domain into "cuboidal" subdomains is arbitrary, but it has to be complete and mutually exclusive.

Despite the partition into mutually exclusive subdomains, the subsequent grids have an overlapped layer of control volumes (CVs) at interfaces. The CVs that protrude from a continuous grid of the block cover the boundary CVs of the neighboring block. The protrusion of the boundary CVs is a regular way of discretization employing the staggered grid to impose the boundary condition on contravariant velocity components. One layer of the extended CVs for the tangential contravariant velocity component is added to the parent part of the block. This layer can produce a discontinuity in gridlines where the interface crosses them. An indeterminacy of the Jacobi matrix of the co-ordinate transformation is associated with the gridline discontinuity. A computation of Christoffel's symbols in the point where the break of gridlines takes place leads to the first order discretization error [9]. A scheme of the decomposed grid interface has been presented in Figure 3.

The exchange data scheme between blocks on their interfaces is based on updating which has to impose sufficient boundary conditions. Details concerning this exchange are lacking in literature. Lilek et al. [10] mention that special care is required to ensure the conservation principles across block interfaces. Thakur et al. [11] analyze the Dirichlet's or Neuman's boundary condition imposed on the pressure correction at interfaces. In this paper the direction of the velocity normal component at the CV face belonging to the interface but situated at the neighboring block is an indicator of a kind of the boundary condition to be imposed on. This direction classifies the suitable cell face as an inlet or outlet face. On the parts of the control surfaces considered as the inlet ones, each block has received 3 velocity components and the pressure gradient component normal to the surface as the boundary conditions. On the surfaces considered as the outlet ones, 2 velocity contravariant components (excluding the normal component), a contravariant component of the deformation tensor along the normal direction and pressure have been taken from the subsequent blocks.

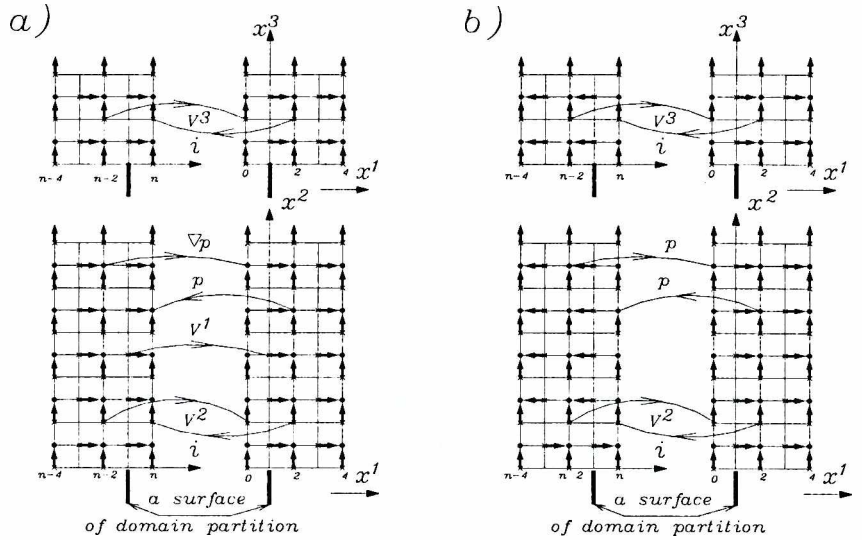

Figure 3. *Scheme of grid interface neighboring blocks and principle of data exchange: a — a case when the flow direction through the interface is the same; b — a case when the flow direction through the interface is the divergent.*

The values of the vector and tensor components exchanged in the presented method are defined in the local curvilinear co-ordinate systems of neighboring grids. The local grid steps of different blocks, which correspond to the same grid segments belonging to the overlapping areas, have to be the same to avoid tensor transforms. It is assumed that all curvilinear steps are equal to one. The signs of the exchanged components need special care as well. They remain the same if there is a consistency of the corresponding co-ordinate directions, or are changed into the opposite ones if the directions of the co-ordinates are opposite.

The decomposed task is not strictly equivalent to the task before the decomposition. The accuracy order of the convection term discretization on the control surfaces is equal to 1. If the grid smoothness is disturbed on the control surfaces, the accuracy of Christoffel's symbol discretization also decreases to achieve the same error magnitude. As the amount of elementary cells lying on the control surfaces is small in comparison with their global number, the consistency order of the discrete solution with the accurate one is equal to 2, but it does not exceed the order of the discretization within the grid.

4. Parallelization

There are some parallelization tools available to compute scientific and engineering problems. Their advantages and disadvantages have been discussed by Foster [12].

The subject of this paper are our own parallelization procedures which have been carried out and applied to solve the 3-D N-S equations with multiblock domain decomposition. In these procedures one computational process in the form

of a complete program unit has been assigned to one subdomain. All processes have been synchronized mutually, employing messages transferred between them by a pointed memory region. Every process has been able to stop, if necessary, in order to wait for the data from the neighboring blocks. This takes place when a given number of iterations has been achieved in this block and its boundary data with the message of its readiness for continuation have been passed. The neighboring block data are loaded, and then continuation of calculations can take place after the process has collected all messages from neighboring blocks. For this kind of a self-control method, an imposition of a global ending condition on all processes together is the main difficulty that one can avoid employing a simple additional process. In the presented calculations, a computer user made a decision, on the basis of accuracy of current iterative results, about ending all processes.

The MPI (Message Passing Interface) libraries have also been used to organize communication to make sure that our codes are correct and to compare both of them. It has been proved that our parallel codes running with various networks of computers are more flexible than that supported on the MPI procedures.

A fundamental notion connected with the parallelization of computations is a parallel efficiency that is defined as:

$$E = \frac{T_{seq}}{nT_{per}},$$

where T_{seq} denotes the CPU time of the computation with a sequential algorithm on one processor, and T_{per} denotes the CPU time of a parallel algorithm on n processors. A lot of efforts have been put into optimization of various parallel codes to achieve a high value of the parallel efficiency [13]. In the ideal case its value is 100%, which means that the parallelization causes an increase in the computing speed to come to its highest expected value. However, the loss of time always occurs with the parallel algorithm due to communication and synchronization, or due to changes in the algorithm required to parallize it, or at least owing to the uneven load of particular processors.

In our case, when the simulation of flows through turbomachinery channels is parallelized, the multiblock domain decomposition depends on a complexity of the channel system rather than on the conditions leading to equalization of every processor load. Therefore, maximization of the parallel efficiency is not the main aim of the parallelization routine for a flow through a system of channels. The CPU time of the parallel computation is always less than that of the sequential computation.

5. Sample Computations

5.1 Flow through the curved ducts

The initial test computations have been carried out for a flow through a strongly curved channel with a square cross-section, investigated by Humphrey et al. [14]. The experiment and computations have been conducted for the Reynolds number

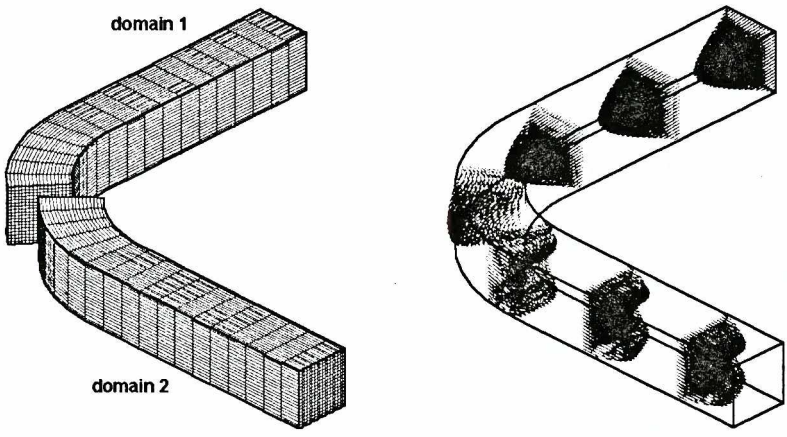

Figure 4. Decomposed channel of the test task and the velocity profiles obtained.

Re = 790, based on the hydraulic diameter and average velocity. At the inlet a fully developed laminar flow in a straight duct has been assumed. Thus, the velocity distribution as a inlet boundary condition has been assessed on the basis of an analytical solution [15] for the case mentioned above. A constant pressure and vanishing velocity gradient components on the outlet surface along the normal to this surface have been imposed at the outlet. The computations have been made in a sequential manner, and after the parallelization by means of the decomposition into 2 symmetrical subdomains whose shapes are the same, as shown in Figure 4.

The calculation has been carried out on grids whose dimensions are 36×31×31 from which the part equal to 14×31×31 is located on the channel arc. The computation time has been reduced to 62% of the time needed for the sequential computations, which gives the parallel efficiency equal to 80.6%. In both cases the first order upwind scheme has been applied to discretize the convection terms. The application of it reduces the differences between the sequential and parallel algorithm due to boundary approximations at the interfaces, as has been mentioned above. A full agreement between the results of the parallel and sequential computations has been obtained. The results of the computation, regarding some velocity distributions, have been presented in Figure 5. An actual and mean velocity ratio depending on the radial location in the middle cross-section has been plotted at the inlet and outlet of the curved part of the duct. The Humphrey's experimental results have been included there for a comparison with those obtained numerically. One can recognize some discrepancy between them that has its origin in the first order accuracy of the discretization of the convective terms.

5.2 Flow through pump channels

The algorithm and code described above have been applied in the numerical simulation of a flow through the first stage of the PM5 centrifugal water pump which was experimentally investigated in 1994 [16]. The stage consists of:

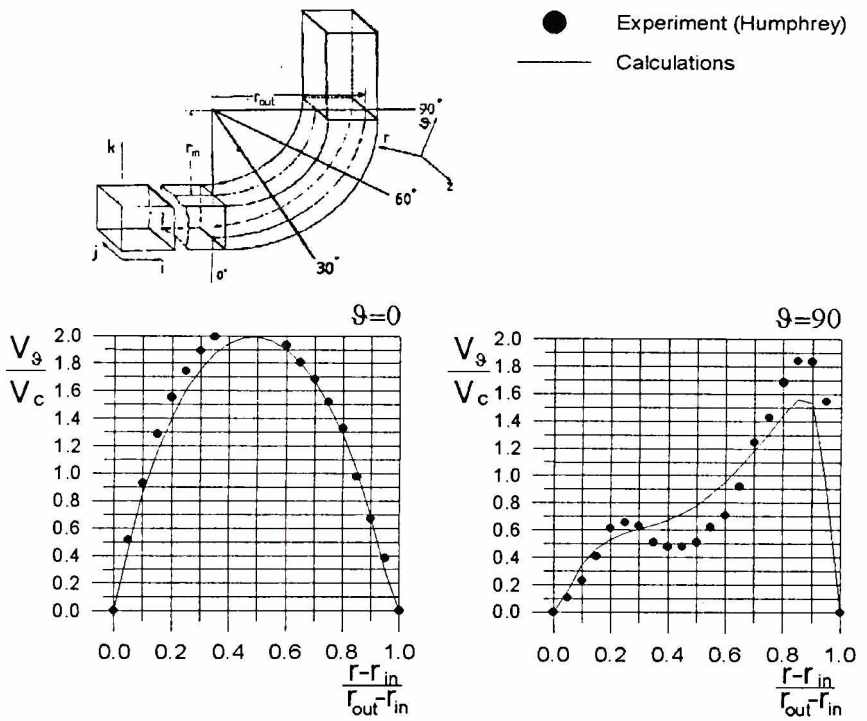

Figure 5. *The distributions of the main velocity component in the middle cross-section: a — at the inlet of the circular part of the duct; b — at the outlet of the circular part of the duct.*

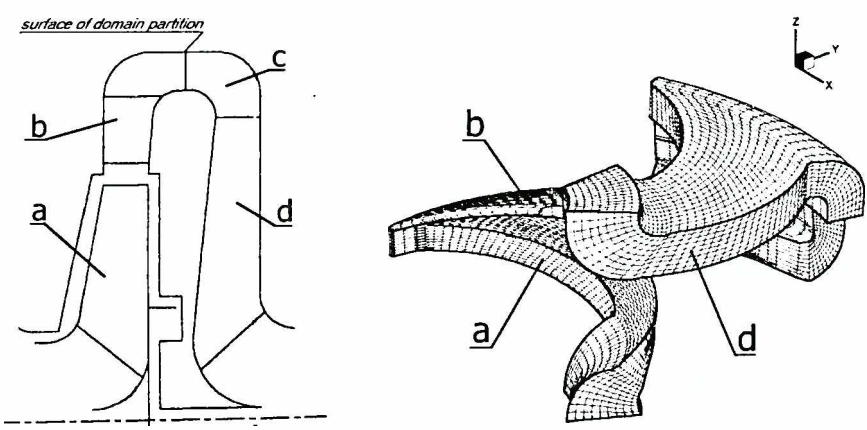

Figure 6. *First stage of the PM5 pump and corresponding grids of channels: a — impeller; b — vaned diffuser channel; c — vaneless U-turn channel; d — vaned return channel.*

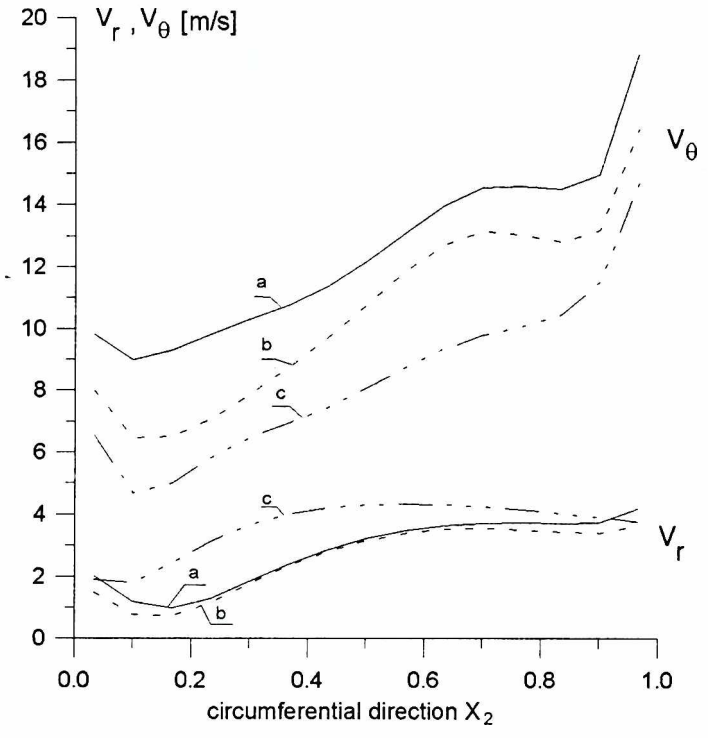

Figure 7. *Distribution of the radial v_r and circumferential v_θ velocity components in the rotating co-ordinate system at the outlet surface of the impeller from the pressure to suction side: a — near the front shroud; b — middle; c — near the back shroud.*

a 7-blade impeller of the diameters 175/355 mm, a 9-vane centrifugal diffuser channel of the diameters 370/500 mm, a vaneless U-turn channel, an 8-vane centripetal return channel of the diameters 500/195 mm. Its meridional cross--section and the computational grids have been shown in Figure 6. The computations have been made for the nominal pump discharge $V = 0.07$ m³/s and the rotational speed of the rotor $n = 24.17$ l/s.

The inviscid flow has been assumed in this version of computation. Moreover, a steady flow model has been used for a strongly unsteady flow due to the rotor--stator interaction. At first, a flow through the impeller has been predicted independently in the sequential manner. The axial uniform velocity distribution has been assumed of the inlet and the uniform pressure distribution has been established at the outlet as the boundary conditions. The outlet has been assumed on the cylindrical surface at the diameter, 15% greater than the impeller diameter.

The computation results of the impeller have been used as the input data for the computations of flow through stationary elements. The circumferential distribution of the velocity components at the impeller outlet in the rotating frame of reference has been shown in Figure 7. Heterogeneity of the velocity distribution can be easily recognized there, especially due to its circumferential component. A rotation of the

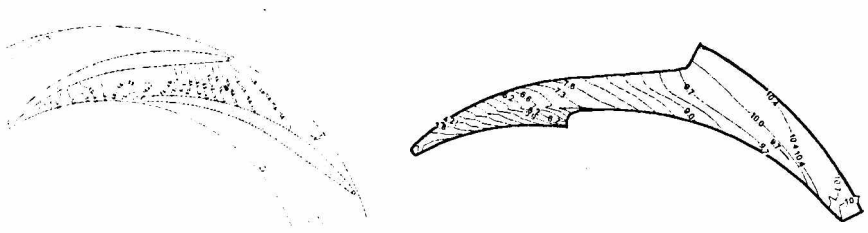

Figure 8. *Isobars on the external wall of the vaned diffuser channel, measurement results (left) and computation results (right).*

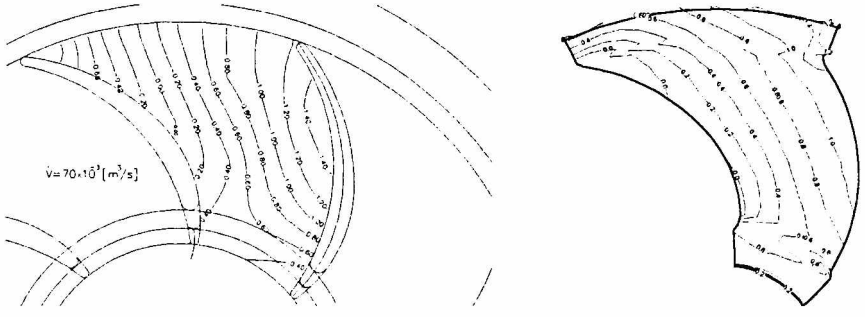

Figure 9. *Isobars on the external wall of the vaned return channel, measurement results (left) and computation results (right).*

heterogeneous field of the velocity entails an unsteady structure of the field in the rotor-stator interaction region and eventually the energy dissipation which is responsible for pressure losses. Such an unsteady flow has been modeled as an averaged steady one. Various averages could be chosen to conserve various physical fluxes [17]. Assessment of the steady velocity for the boundary condition at the inlet surface of the stationary channels is essential to predict accurately the pressure increase in the stage. The inlet surface of the stationary calculation domain is the physical outlet of the impeller. All velocity components at the inlet to stationary channels have been estimated by average components of the rotational velocity at the impeller outlet. The rules of calculation of the averages are different for different components. In the cylindrical co-ordinate system, the radial velocity component has been estimated from the formula:

$$v_{r2}(z) = \frac{1}{2\pi}\int_0^{2\pi} v_{r1}\, d\theta$$

that conserves the mass flow rate, whereas the circumferential and axial components have been averaged as follows:

$$v_{\theta 2}(z) = \frac{1}{2\pi\, v_{r2}} \int_0^{2\pi} (v_{\theta 1} + u) v_{r1} d\theta,$$

$$v_{z2}(z) = \frac{1}{2\pi\, v_{r2}} \int_0^{2\pi} v_{z1} v_{r1} d\theta$$

conserving the momentum in the absolute reference system. In the above averaging formulae, subscripts denoted by 1 concern the components in the rotating frame of reference; 2 — average components in the absolute system; u means the circumferential velocity of the impeller. The value of the pressure has been imposed at the outlet of stationary channels as the boundary condition.

The parallel computations have been carried out for stationary elements of the pump stage. The domain decomposition has been made by means of the division of the vaneless U-turn channel by the plane perpendicular to the pump axis (Figure 6). Owing to different numbers of vanes in the vaned diffuser channel and in the vaned return channel, the task should be solved in a large domain, which would consist of all stationary vane to vane channels treated as subdomains. Such a decomposition leads to a partition into 17 subdomains and causes the task to require large computer resources. The assumption about the periodicity in the vaneless part of the channel allows us to reduce the calculation domain to a combination of 2 blade to blade channels. Different periods in different subdomains are supposed to characterize the periodicity on both sides of the partition plane. On the inlet side the period equal to $2\pi/9$ has been established, whereas on the outlet side the period equal to $2\pi/8$ has been assumed. The values of the periods follow from the circumferential width of the blade to blade channels on both sides of the division plane. Fulfillment of both kinds of the periodicity condition entails an existence of an axisymmetrical flow on the partition plane, which is confirmed by the experimental investigations. Two subdomains and two periodical phantoms of the narrower subdomain have been assumed to organize a boundary swap.

The numerical results have been put together with the experimental data in Figures 8 and 9. The pressure distributions on the external walls of the vaned channels have been shown. Comparing the obtained results with the experimental ones, one can see a good agreement between them as regards pressure gradients rather than absolute values, despite the fact that an inviscid flow model has been employed.

In Figure 10 the values of averaged pressures at the control surfaces are shown. The same pressures have been assumed at the outlet surface according to the computational scheme. The connection lines between the measured and calculated pressure values on the presented surfaces have only an illustrative character. The discrepancies between the measured and calculated pressure rises can be especially observed for the pump impeller. This is probably caused by the numerical dissipation of the first order upwind scheme applied in the numerical code. An improvement of this scheme is anticipated in the nearest future. The relative total

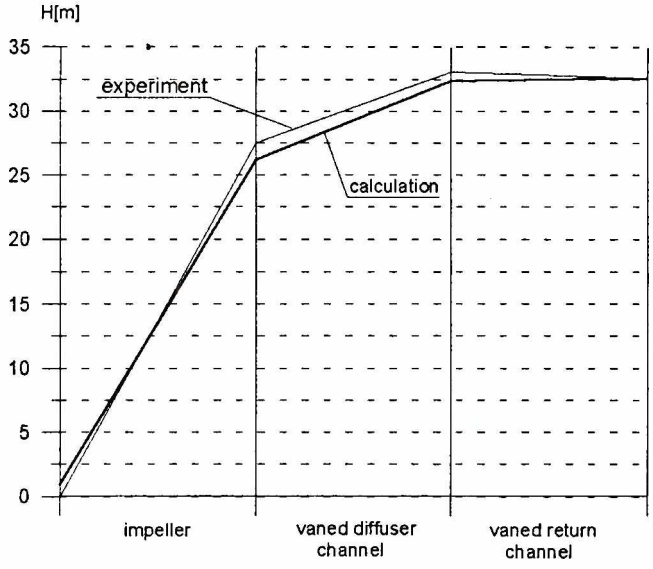

Figure 10. *Values of averaged pressures at the control surfaces.*

difference in the pressure rise of the pump consisting of three elements (impeller, centrifugal vaned diffuser channel, centripetal vaned return channel) is approximately 3% and can be considered as a satisfactory result.

6. Conclusions

The domain decomposition has turned out to be an efficient method of determination of 3-D flows through the water pump channels characterized by a complex geometry. The parallelization of computations, based on the domain decomposition, leads to reduction of computing time. The maximization of the parallelization efficiency is limited by decomposition methods which follow from the complexity of the channel geometry.

Our codes, based on the pressure correction algorithm and parallelized by means of own message passing system, foresee very accurately the velocity and pressure distributions of the viscous flow through a curved channel and the inviscid flow through channels characterized by a complex geometry in the centrifugal pump stage. These satisfying results have been obtained despite the fact that significant simplifications have been introduced into the flow model, especially as far as a flow through the pump stage is concerned. This is mainly connected with the averaging procedure at the control surfaces between rotating and stationary pump channels. Therefore, further investigations aiming at more precise determination of flow structures and estimation of a pressure increase in the pump stage are needed. Two issues connected with this seem to be the most urgent ones. The first one refers to an application of turbulence closure models in computations carried out on decomposed domains. The second one concerns studies on estimation of pressure losses connected with the stator-rotor interaction, which should be undertaken.

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