DNS and RANS/LES-Computations of Complex Geometry Flows Using a Parallel Multiblock Finite-Volume Code

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The parallel capabilities of today's workstation or PC clusters have made possible economical numerical studies of turbulent flows on the base of unsteady formulations in applications to both simplified and complex geometry configurations. Well-known techniques are Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES). However, true or full resolving DNS remains to be extremely time-consuming for Reynolds numbers of more than 10^4. In this situation many authors undertaken attempts for underresolved DNS studies, with surprisingly good results in specific cases. A huge amount of recent contributions was devoted to applications of Large Eddy Simulation (LES) that can be used at much higher Reynolds numbers than DNS. In case of wall-bounded flows, the major difficulties and uncertainties of LES are associated with the treatment of the near-wall layers. Last years, hybridizations of the Reynolds-averaged Navier-Stokes (RANS) approach with LES become more and more popular (Spalart, 2000). Among various techniques, Detached Eddy Simulation (DES) suggested initially for prediction of massively separated turbulent flows is of special interest. The main idea of DES is to entrust the near wall layers to a RANS model, and the region far away from the wall to LES. A comprehensive description of the state-of-the-art in DES of massively separated flows is given by Strelets (2001). Recently promising attempts have been done to perform DES-like computations of strongly turbulent Rayleigh-Benard convection (Smirnov, 2002).

The *first part* of the present contribution covers peculiarities of parallelization of an in-house 3D steady/unsteady Navier-Stokes code SINF (Supersonic to INcompressible Flows). Being under permanent development since 1992, this code is based on the second-order finite-volume spatial discretization technique using the cell-centered variable arrangement and body-fitted structured (matching or non-matching) grids. The ideas of the artificial compressibility method or the compressibility scaling technique are employed to compute both incompressible and compressible fluid flows. The pseudo-time evolution problem is solved using implicit schemes such as the approximate-factorization scheme or the Gauss-Seidl plane/line relaxation schemes. Dealing with unsteady flows, the pseudo-time iterations are performed for each physical time step. Three-layer second-order scheme was implemented for physical time stepping. Third- and second-order upwind schemes are employed for convective flux evaluation. For low-speed flows, the solver uses a generalized Rhie-Chow interpolation to avoid de-coupling between velocity and pressure. CUSP-type schemes were implemented to handle shock regions of transonic flows. High- and low-Reynolds number versions of several one- and two-parametric differential turbulence models are available for simulation of turbulent flows in the RANS mode. In 2000-2002 the code capabilities were extended to apply the LES and DES techniques.

The parallelization of the code is based on the domain decomposition according to block-structuring of grids, an SPMD (Single Program Multiple Data) strategy, and the MPI standard (Message Passing Interface Forum 1995). The main peculiarities of parallelization concern the data exchange at the interface regions between logical neighboring subdomains. In the non-

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parallel (prototype) version of the code the boundary updating at the interface of neighboring blocks (after completion of an iteration step) is done via computations within a “virtual” block. This virtual block is formed from near-interface layers of connecting physical blocks, with copying all the data needed for computations of fluxes through the interface. Note that the virtual block concept adopted in the code SINF ensures the conservation of the fluxes at the interface and facilitates solution of many problems associated with the use of non-matching grids and/or with complicated conjugate heat/mass transfer tasks. In the prototype version of the code the virtual block computations are performed sequentially, interface by interface, using the same storage. In order to achieve a high efficiency of parallelization and to avoid the use of a large single master process, copies of near-interface layers of the physical blocks are created in a special process, and the latter performs the interface updating in the same manner as in the serial mode. It is illustrated in Figure 1.

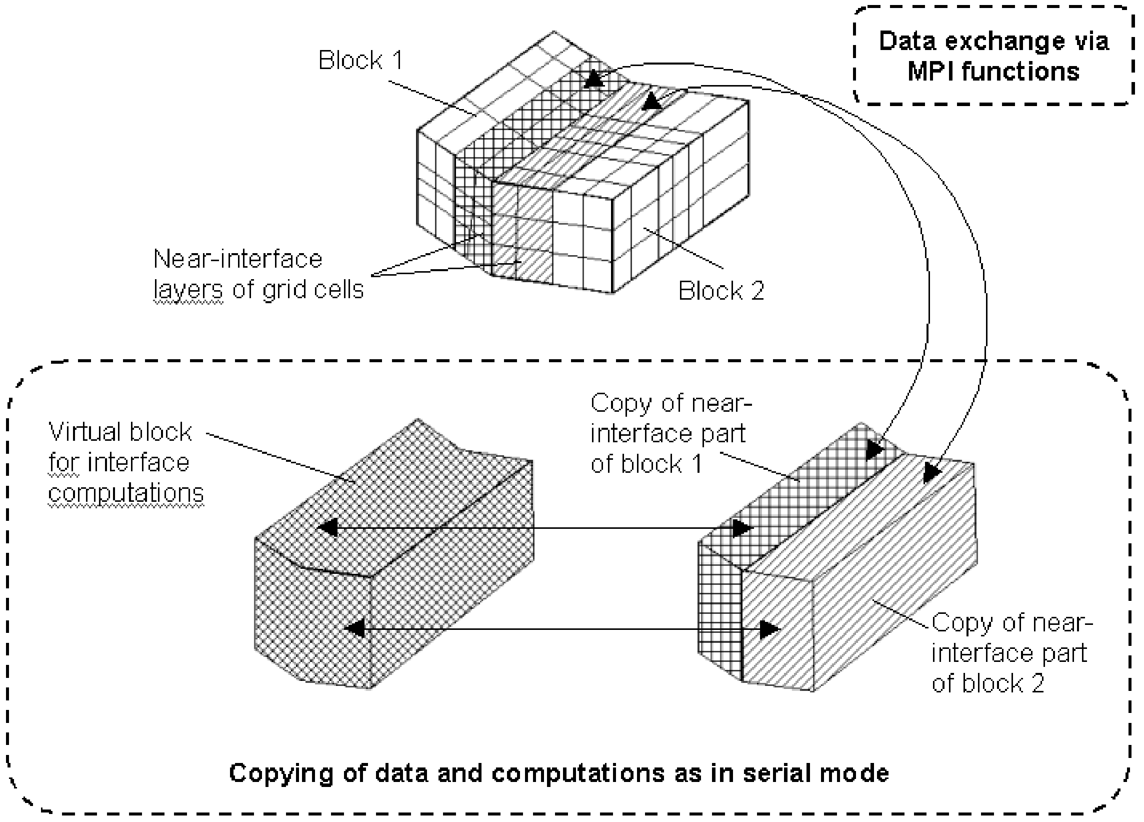

Fig. 1. Scheme of data exchange in the parallel version of the code SINF.

To date, our experience in using the parallel version of the code was limited by using PC clusters of 24 processors or less. For most flow configurations considered (using grids with size of 0.6 to 2.4 million computational cells), the parallelization efficiency is higher than 0.8.

The *second part* of the present contribution covers several examples of 3D industrial flows computed on the base of DNS and RANS/LES. The first example concerns simulation of unsteady turbulent melt convection in a real-geometry crucible of a Czochralski (CZ) system for silicon single-crystal growth. It is known that low-frequency unsteady 3D oscillations of the melt observed for industrial-scale CZ systems result in striations of impurity (oxygen) concentration in the crystal and in significant melt temperature fluctuations affecting the crystal defect formation. Typically, velocity fluctuations are comparable or even larger than the local average velocity, and the turbulent transport is mainly controlled by large-scale eddies, the statistical effects of which are very difficult, if possible, to predict on the base of RANS turbulence models. Recently LES and RANS/LES-computations were performed for an industrial CZ furnace using a non-parallel version of the code SINF (Evstratov et al., 2002). A computational grid covering the melt convection domain was of about 100,000 cells. With this grid, the thermal unsteady state of the melt and heat transfer features were predicted quite well, as compared with the measurements done for this furnace. However, a qualitative disagreement with experimental data was observed for the oxygen content versus the crucible rotation rate. To discover the reasons of the disagreement, direct numerical simulation of silicon melt turbulent convection at a Rayleigh number of about 10^6 (reduced as compared with the industrial prototype) has been performed with the parallel SINF on a grid of next to one million cells. Results obtained for the velocity and temperature fields are close to those of RANS/LES obtained with a coarser grid. The most remarkably, however, that now the tendency in the oxygen content versus the crucible rotation corresponds to the experimental observations.

The second example considered is turbulent flow through a single row of square bars with a pitch three times the bar side. The Detached Eddy Simulation technique based on the one-equation Spalart-Allmaras turbulence model (Sterelts, 2001) was used that allowed predictions of 3D vortex structures of the flow and temporal oscillations of the drag and lift forces acting on the bars. Assuming the bar cascade is unlimited both in the pitchwise and spanwise directions, periodicity conditions are imposed on corresponding planes. It has been established that the computational domain should cover at least two pitches of the cascade. Computations performed with the parallel SINF on grids of about one million cells are compared with available experimental data and with 2D unsteady RANS results obtained using the same code.

The third problem concerns predictions of separated flows in exhaust diffusers of gas turbines. Typically, a gas turbine exhaust diffuser has inner struts that play several roles in the construction. To minimize pressure losses in the diffuser, profiled strut covers are used in the majority of machines. At off-design conditions, the flow after the gas turbine last stage has a considerable swirl that results in a high incidence and in a massive separation of flow from the profile. When performing numerical simulations of 3D separated flows one usually tries to reduce the problem dealing only with one sector of the diffuser and imposing periodicity boundary conditions in the circumferential direction. It is known, however, that in real unsteady massively-separated flows there are pronounced deviations from the circumferential periodicity despite the rotational symmetry of the geometry. We present a study of time-dependent deviations from the circumferential periodicity using an exhaust diffuser model with six real geometry profiled struts. The whole 360-degrees model of the diffuser is considered. Direct numerical simulation with no-turbulence model was performed at a Reynolds number of 10^3 using a grid of 2.4 million cells. It has been established, in particular, that there is a considerable phase shift in leading-frequency oscillations of velocity at compatible monitoring points placed in the separation zones of different struts. However, the statistics of separated flow oscillations is close to that obtained for a 60-degrees model with periodicity boundary conditions imposed.

The last example is also related to turbomachinery applications and concerns a film cooling configuration. Film cooling is considered as the most efficient blade-cooling mechanism employed in gas-turbine technology. In most film cooling applications, the coolant flow is injected in the same direction as the main flow (streamwise injection). In the region of the main-stream/coolant-jet mixing, the film cooling flows are highly unstable, and turbulence is considerably anisotropic. Since RANS calculations fail to reproduce important unsteady flow phenomena, there is a strong motivation to try RANS/LES-techniques for getting a reliable tool for predictions of film-cooling effectiveness under real operating conditions. We present an initial experience in RANS/LES applications to film cooling problems. A particular configuration, recently studied experimentally in (Burd et al., 1998), is considered. The computational domain covers a part of main stream, an inclined hole (used for the coolant supply) and a plenum, so that the real geometry of the experimental rig is well reproduced. RANS/LES-computations on a grid of about 600,000 cells were performed using a one-equation turbulence model based on the transport equation for the turbulent kinetic energy of unresolved motion (Smirnov, 2002). The computations have reproduced the most important features of the

3D velocity field measured in the experiments. However, results for the thermal field are not satisfactory, and very sensitive to numerical details.

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