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Supercomputer Simulation of MATIS-H Problem

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A supercomputer simulation of the benchmark MATiS-H problem is considered. A high-resolution CABARET code is applied for solving Navier-Stokes equations in the framework of the Monotonically Integrated LES approach for the MATiS-H problem. The code is based on a generalisation of low-dissipative, low-dispersive and non-oscillatory CABARET scheme to hybrid topology meshes in the supercomputing framework. The solutions for the time-averaged fields are reported. These show a relatively small sensitivity to the grid density. Comparison with the experiment data available is provided.

Keywords: Navier-Stokes equations, parallel computation, modelling, Cabaret method.

Introduction

For modelling of unsteady flow mixing in the MATiS-H rod-bundle configuration with a spacer grid [1], the Monotonically Integrated LES (MILES) approach of Fureby and Grinstein [2] is used. Similar to other Implicit LES techniques, this approach does not include any explicit sub-grid-scale closure. The sub-grid-scales are modelled implicitly on the assumption that the shock-capturing and the good linear wave properties of the numerical scheme are most important for accurate transport of localised vortical structures embedded in a weak background vorticity that has direct relevance for the correct representation of turbulence energy cascade. Indeed, the capability of capturing sharp velocity gradients for smallest resolved scales leads to the emulation of high-wavenumber end of the inertial subrange region characterised by thin filaments of intense vorticity. The above assumption was indirectly confirmed in the work of Fureby and Grinstein who showed that a MILES model of sub-grid-scale closure can be rearranged to a non-linear dissipation filter form typical of the classical LES approach and leads to encouragingly accurate results for the solution of several shear and channel flow problems in comparison with the LES solutions obtained based on explicit sub-grid-scale modelling. For the MILES approach, the use of high-resolution shock-capturing numerical methods that are also low dissipative and low dispersive is important. The CABARET scheme is one example of such methods. CABARET stands for Compact Accurately Boundary Adjusting high-REsolution Technique which is an original computational method for convection/advection dominated flow modeling that has been developed over the years, starting from a 1D advection equation to a highly parallelized 3D unstructured Navier-Stokes code that allows one to conduct eddy-resolving simulations with correct capture of inertial range of turbulent kinetic energy spectra up to very high frequencies. Characteristic features of CABARET include its low dispersion and low dissipation. For linear advection the dispersion error of the CABARET method is as low as that of fourth order finite-difference schemes, yet it is shock-capturing, robust for non-uniform grids, fast and as simple for implementation as conventional shock-capturing finite-volume schemes, e.g., Total Variation Diminishing (TVD) Schemes. In comparison with the latter, the dispersion and dissipation errors of CABARET scheme are a few orders of magnitude lower. Up to present, CABARET algorithm has been found very efficient for a number of Computational Fluid Dynamics (CFD) problems including the modeling of forced turbulence, high-speed jet and airfoil flows and also

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turbulent flow mixing in a T-Junction configuration corresponding to a OECD/NRS blind test exercise [3–6]. Another important property of the CABARET method is the compactness of its computational stencil. This makes CABARET scheme very affordable for supercomputing because of the stencil simplicity and low communication overheads. In the current work, for most flexible treatment of the complex spacer grid geometry, the previous CABARET code that has been available only for the hexagonal grid topology has been extended to hybrid meshes.

1. The Governing Problem Formulation and Parallel Numerical Solution Procedure

The unsteady flow in the MATiS-H configuration is modelled by the system of slightly compressible Navier-Stokes equations:

$$
\begin{aligned}
&\frac{\partial p}{\partial t}+\rho_0 c^2\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)=0\\
&\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}+\frac{1}{\rho_0}\frac{\partial p}{\partial x}=\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)\\
&\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}+\frac{1}{\rho_0}\frac{\partial p}{\partial y}=\nu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)\\
&\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}+\frac{1}{\rho_0}\frac{\partial p}{\partial z}=\nu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right).
\end{aligned}
$$

Here ρ_0 – density, c – sound speed, x, y, z – coordinates, t – time, u, v, w – velocity vector components, ν – kinematic viscosity, p – hydrostatic pressure.

Laminar inflow boundary conditions are specified at about 10 hydraulic diameters upstream of the space grid. The meanflow parameters for the inflow input, as well as the initial conditions are obtained from a precursor k-e solution of Reynolds-Averaged Navier-Stokes (RANS) equations on the same grid. The numerical solution procedure of the unsteady flow equations consists of 3 phases [3]. Phase 1 and phase 3 correspond to the conservation predictor and corrector steps of the CABARET scheme and stand for the conservation balance laws. Conservation flux of the CABARET scheme is calculated at phase 1 and phase 3. Phase 2 is a characteristic decomposition step. During this stage, the one-dimensional Riemann variables are defined for each face normal projection. The characteristic values at the new time level are obtained from a second-order extrapolation according to the characteristic directions.

The values of the Riemann variables computed are truncated if found to lie outiside the allowable min/max in accordance with the discrete maximum principle. The algorithm is implemented in a highly scalable hybrid mesh framework based on a custom-made MPI parallelisation with a very good efficiency of up to 2,000 computational cores for problem sizes up to several million cells.

2. Parallel Decomposition and I/O Details for Supercomputing

Because of the large-eddy-resolving nature of simulations typical of the MILES approach, LOMONOSOV Supercomputing Facility of Moscow State University has been used. In parallel, several calculations are performed on a dedicated computer cluster at the Moscow Institute of Nuclear Safety (IBRAE) of Russian Academy of Science. The use of a massively parallel computational environment in the framework of the complex grid geometry of MATiS-H required an additional upgrade of the CABARET code as outlined below. The hybrid mesh model generated with a commercial grid generation package has been exported to OpenFOAM. The latter is a free-source software package that includes a grid decomposition kit that is fairly reliable for parallel computations. Despite the general robustness of this software, we had some problems during the processing of the models, the size which exceeds 20×10^6 cells as discussed below. During the mesh decomposition over 1000 processors, 8 files in each of 1000 directories have been created, and because of the time-transient calculations during the post-processing stage this can quickly end up with 1,000,000 files which is far above the admissible limit of the number files for a supercomputer file system. Hence, we implemented special Fortran procedures to relax the load on the file system and simplify the post processing. The parallel decomposition for the 4.5×10^6 and 13.1×10^6 models has been conducted with METIS. For the model of 47×10^6 cells, ManualFile is used. For this decomposition, the scalability of the 47×10^6 model up to 1800 computational cores is about 75% of the linear speed-up rate, which is acceptable in our application. Figure 1 (left) shows a cross-section of the computational core enumeration for the ManualFile method. For calculations with 1800 cores, the number of cores along the stream is 72.

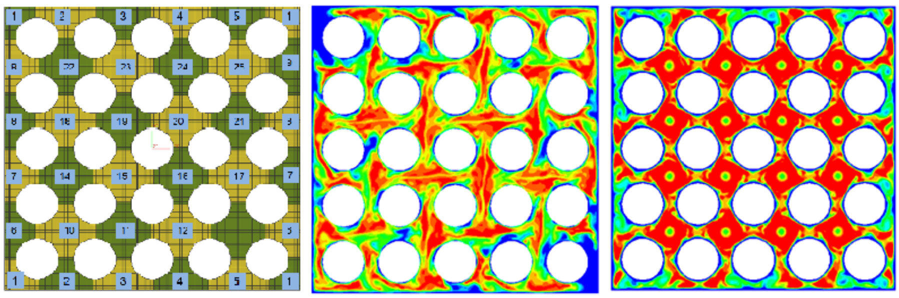

Figure 1. Core enumeration in the cross-section and snapshot of the axial velocity (z=4.0dh)

3. Numerical Result Mesh Comparison for the MAIS-H Test

Figure 1 (center and right) shows the axial velocity contours in the cross-sectional snapshot z=4.0dh for the split-type and swirl-type geometries. Numerical comparison of the predicted velocity field distribution with the experiment is shown in Fig. 2. Figure 2 also shows the results of the mesh sensitivity study.

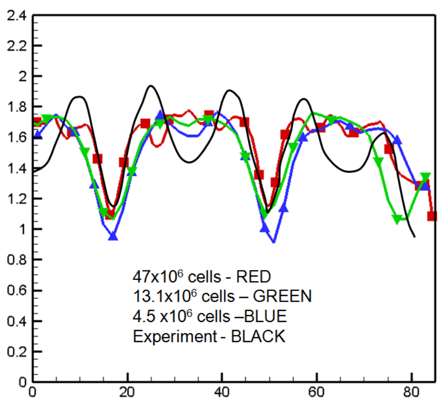

Figure 2. Axial velocity comparison for swirl, y/p=0.5 and z=0.5Dh with different meshes (grids=4.5, 13.1, and 47x106 cells)

The numerical solution generally shows an encouraging agreement with the experiment. For a more correct representation of mixing effects, resolving the scales could also require a fine computational grid further downstream of the mixer grid, as well as in its vicinity.

Conclusion

A hybrid-mesh modification of the MILES CABARET method has been applied for the MATiS-H problem. The computational results show only a small grid sensitivity for the grid resolutions studied ($4.5 - 47 \times 10^6$) in terms of the means velocity distributions. Lomonosov supercomputer facility has good scalability of up to 1800 computational cores.

Acknowledgments

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