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PRESENTATION OF NEW LES CAPABILITY OF ADREA-HF CFD CODE

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Abstract: The ADREA-HF is a general purpose Computational Fluid Dynamics (CFD) code, with extensive use in environmental applications. In the current work, the task of adding and testing the Large Eddy Simulation (LES) capability is presented. After simulating a fully developed channel flow, a simple street canyon geometry is examined. Flow field and Reynolds stresses' results are compared with experiment and other LES and Direct Numerical Simulations (DNS). The accuracy and efficiency of the modified code is presented along with comments about the applicability of LES in urban flows.

Key words: *CFD, Large Eddy Simulation, ADREA-HF, urban street canyon.*

INTRODUCTION

Nowadays, CFD calculations like atmospheric dispersion modelling and urban flows become more demanding, as the computational power increases. New techniques, like the LES, previously used mainly for research, emerge as a promising alternative way of calculating atmospheric flow and pollutant dispersion. Compared to Reynolds Averaged Navier-Stokes (RANS) methodology, LES uses a natively transient approach, solves most of the turbulence, is capable of predicting the intermittent character of the flow and provides detailed information for the turbulence statistics, but computationally it is orders of magnitude more expensive and requires usually unavailable accuracy of boundary conditions data. Even if RANS and LES are fundamentally different, they end up in similar formulation of the main discretized equations, thus making it possible in most cases to use a pre-existing RANS code to develop a new LES one and having a single program for both techniques.

The ADREA-HF (Bartzis, J. G. *et al.*, 1991, Venetsanos, A. G. *et al.*, 2010) is a flexible CFD code that has been extensively used, among others, in calculation of urban flows, atmospheric pollutant dispersion modelling and hazardous releases safety assessment, in arbitrary complex geometries. It is currently under upgrade, with recent additions of a highly modern and intuitive pre-processing and post-processing Graphical User Interface (GUI), various numerical options, combustion calculations ability, handling of arbitrary number of species and finally an efficient parallel solver and LES, which are detailed here.

The test cases that are chosen to evaluate the LES model of the code are the classic fully developed channel flow that is a very good trial for LES and essentially a two-dimensional (2D) street canyon, which is one of the most basic urban flows. Several street canyon LES studies exist (Walton, A. and A. Y. S. Cheng, 2002, Baker, J. *et al.*, 2004, Li, X. X. *et al.*, 2008), usually comparing LES with reduced scale experimental data. From those studies, mainly the actually intermittent character of the street canyon flow is revealed.

METHODOLOGY

Governing equations

In LES, the large turbulent scales containing most of the energy are resolved explicitly, while only the Sub-Grid Scales (SGS) containing a small fraction of the energy are modelled. A spatial filtering is applied to every variable of the flow field, decomposing it into a resolved (of filtered) component and an SGS component. The filtered governing equations neglecting the terms not used in this study, take the form (Jiang, X. and C. H. Lai, 2009):

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial(\tilde{\tau}_{ij}^l + \tau_{ij}^R)}{\partial x_j}\ ;\ \tilde{\tau}_{ij}^l + \frac{2}{3}\mu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij} = 2\mu\tilde{S}_{ij}\ ;\ \tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) \tag{2}$$

$$\bar{p} = \bar{\rho}r\bar{T} \tag{3}$$

The instantaneous variables here are space-averaged and not time-averaged, like in RANS, while the tilde denotes density weighted Favre-averaging. $\tilde{S}_{ij}$ is the instantaneous rate-of-strain tensor, r is the gas constant, $\tilde{\tau}_{ij}^l$ is the instantaneous shear stress tensor due to molecular forcing (l is for laminar) and $\tau_{ij}^R = -\bar{\rho}\widetilde{u_i u_j} + \bar{\rho}\tilde{u}_i\tilde{u}_j$ is the residual stress tensor due to the subgrid turbulence, modelled using the classical Smagorinsky subgrid scale model, as:

$$\tau_{ij}^R + \frac{1}{3}\tau_{kk}\delta_{ij} = 2\mu_t\tilde{S}_{ij}\ ;\ \mu_t = \bar{\rho}(C_s\Delta)^2\sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}\ , \tag{4}$$

where C_s is the Smagorinsky constant, with the most-commonly used value of 0.1. The term $\frac{1}{3}\tau_{kk}\delta_{ij}$, which is usually negligible compared to thermodynamic pressure (Erlebacher, G. et al., 1992), is incorporated into the filtered pressure. The filter-related Δ is taken as $\Delta=V^{1/3}$, where V is the volume of the computational cell. Near the wall, the length scale $C_s\Delta$ is replaced from κd, where $\kappa=0.41$ is the Von Karman constant and d is the distance from the closest wall.

Numerical method

The resolved-scale equations of the mathematical model are solved with the finite volume method on a staggered Cartesian grid. The discretization equations are presented in Bartzis, J. G. *et al.* (1991). Arbitrary complex geometry is plunged into the grid with the use of porosities (Venetsanos, A. G. *et al.*, 2010). The pressure and velocity equations are decoupled with the use of the ADREA/SIMPLER algorithm, described in the appendix of Kovalets, I. V. *et al.* (2008). The code also features automatic time step handling and a variety of convective terms discretization schemes. For more about the numerical formulation of ADREA-HF, the user is referred to Venetsanos, A. G. *et al.*, (2010). For the current LES simulations, a deferred correction central scheme (Ferziger, J. H. and M. Perić, 2002), which provided high numerical stability and good accuracy, was chosen for the convective terms discretization.

ADREA-HF is parallelized in shared memory architectures with the use of OpenMP directives. The code has various methods for the solution of a linear system, some of which are presented in Kovalets, I. V. *et al.* (2008). For the current runs, the Krylof subspace method BiCGstab (Saad, Y., 2003) was used, with the recently implemented additive Schwarz preconditioner (Saad, Y., 2003): The matrix of unknowns of the linear system is split in one-level overlapping diagonal blocks, and the ILU(0) preconditioner is applied to each one. Both the creation of the preconditioner and the solution of the preconditioner system are done in parallel. The speedup with the use of 2 processors was up to 1.7 and with 4 processors up to 2.5.

Boundary/initial conditions and test cases set-up

The fact that LES is a natively unsteady methodology designed to calculate explicitly most of the turbulence, makes it very demanding regarding the initial and boundary conditions. Initial conditions must be such that they can provide/produce turbulence and boundary conditions should change in time in a turbulence-consistent way, which is very difficult to achieve. In the case of fully developed channel flow, a good initial condition is a large perturbation superimposed on a realistic mean flow (Piomelli, U., 2001) and that technique was used in this study. A good boundary condition for the streamwise and spanwise directions is the cyclic boundary condition, which accounts for consistent turbulence preservation and makes it possible to simulate directly the fully developed flow of infinite plates on a small domain, with the cost of an increased computational time. The cyclic boundary condition was implemented by calculating the boundary momentum values with second-order accurate linear interpolation between the facing boundary cells' values just before the end of each iteration. In the current work, an inlet mass flow correction was used in order to control the flow and retain a prescribed bulk Reynolds number, in a way similar to that described from Denev, J. *et al.* (2004).

Fully developed channel flow

The classic DNS simulation of Moser, R. D. *et al.* (1999) with Reynolds number based on wall friction velocity Re_τ=395 was chosen as a reference case. The LES computational domain is the same as in the DNS, namely 2π, π, and 2 meters in the streamwise (x), spanwise (y) and perpendicular-to-the-walls (z) directions respectively, discretized as a 30x50x60 grid, non-uniform in the z direction. Simulations were also performed with the commercial code STAR-CD, in order to gain experience and have another LES to compare with. Based on STAR-CD guidelines, first of all a RANS computation was performed in the same grid using a low-Reynolds k-ε turbulence model in order to examine the time scales involved and the adequacy of the grid resolution. The LES time-advancement step was chosen to be less than the k-ε time scale near the wall and also to satisfy the numerical criterion that a typical Courant (CFL) number should be less than 0.3. In ADREA-HF the automatic time-step selection was active, along with the criterion to keep the highest local CFL number throughout the domain less than 0.3, which resulted in an average time step slightly higher than that of STAR-CD. In STAR-CD the flow is controlled by keeping the pressure drop constant along the canyon. Cyclic boundary conditions are used in free boundaries and no-slip conditions on the walls for both codes. The first grid point near the wall is placed at z^+=1, which is the suggested value for well-resolved LES with no wall functions (Piomelli, U., 2001). Δx^+ is 83 and Δy^+ is 25, also within the suggested values (50-150 and 15-40 respectively). Smagorinsky constant was fixed to 0.065, which is the proposed value for channel flows (Ferziger, J. H. and M. Perić, 2002).

The equations were integrated in time until 20 s (over 60 passes from the domain), well after a statistical steady state was reached, as it can be seen a posteriori from the time series of the field variables. Then the run continued for another 30 s (50 s total simulation time) in order to provide statistically averaged values to compare with DNS data. In ADREA-HF, the statistics module that was incorporated uses running sums of variables of interest to calculate the statistics on the fly. After the end of the run, a space averaging (which is somehow equivalent to additional time averaging) in the constant-z planes was also performed for each variable of interest, in order to have better statistical averages, since the problem is actually one-dimensional. LES runs reported here need about 1 to 2 days in one processor core of a modern PC, while the RANS run on the same grid needs less than 1 hour.

Street canyon

Following the encouraging results obtained in channel flows, street canyons' LES simulations with ADREA-HF were performed. The Li, X. X. *et al.* (2008b) water channel experiment was chosen to compare with, because it had a Reynolds number that could ensure turbulent flow, while being low enough for full-LES to be performed. Also it had a sequence of identical street canyons, which makes the use of the very practical cyclic boundary conditions fairly acceptable. Other advantages of the particular experiment include the measurement of Reynolds stresses, which are very useful variables for LES validation, and the fact that the authors have performed their own LES simulations (Li, X. X. *et al.*, 2008) that could also be used to compare with ADREA-HF.

The classic street canyon of aspect ratio 1 was modelled. The Reynolds number based on the free stream velocity and the building height was 12000, as in the experiment. The computational domain was the same as the one used from Li *et al.* (2008) at their own LES simulations and is shown in Figure 1. Along with the use of cyclic boundary conditions, it represents an infinitely long street canyon in the spanwise direction that is repeated in the streamwise direction. The bulk Reynolds number was kept constant with mass flow correction technique, as stated earlier. On top of the domain the symmetry plane boundary condition (zero vertical velocity component) is applied, as in Walton, A. and A. Y. S. Cheng (2002). This boundary condition locally suppresses turbulence, but as it can be seen a posteriori, that does not affect the in-canyon flow patterns. The Smagorinsky constant was kept to its default value and the total grid points were limited to about 150000 in this first attempt to see if the LES of ADREA-HF can capture the basic characteristics of the street canyon flow. The in-canyon non-uniform grid has an expansion ratio of 1.1 and the cell centres close to the solid surfaces have a non-dimensional distance x^+ or z^+ of about 1.

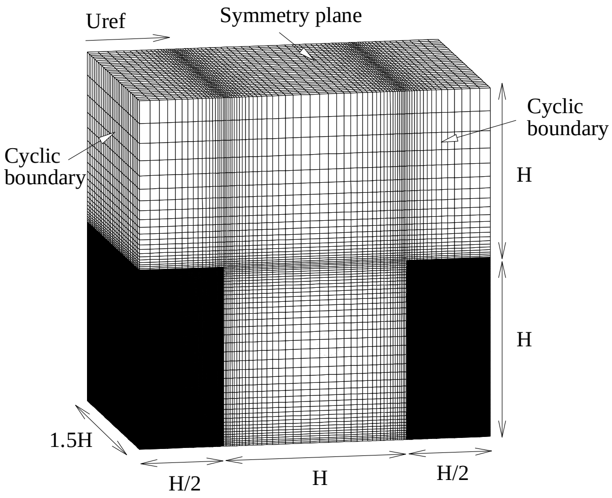

Figure 1. Geometry, grid and boundary conditions for the street canyon LES simulation.

An initial perturbation to the mean velocity field is not applied here, since the presence of the notch is enough to provoke turbulence. For the flow and turbulence to achieve statistically steady state, the LES was integrated for 100 dimensionless time units H/U_{ref}, as in Li, X. X. *et al.* (2008), with an average time step of about 0.003 H/U_{ref}, assuring that the CFL number never exceeded 0.5 in any cell of the domain. The simulation continued for 150 more dimensionless time units for statistical analysis. Time-averaged results are also space-averaged along the spanwise direction before being plotted.

RESULTS AND DISCUSSION

Fully developed channel flow

In Figure 2 the velocity profile of the bottom half of the canyon is presented ($U^+=U/u_\tau$, $z^+=zu_\tau/v$, where u_τ is the friction velocity and v is the kinematic viscosity). Both LES codes captured the general shape of the curve, but there are quantitative discrepancies. STAR-CD seems to better capture the near-wall region, but then departs from the DNS profile overestimating U^+, while ADREA-HF stays on average closest to the experimental curve. Sensitivity tests performed with ADREA-HF revealed that with smaller C_s results get better near the wall, but worst away from the wall. Indeed, a major drawback of the Smagorinsky model is the non-universal value of C_s, which makes many scientists prefer more complex models like the dynamic Smagorinsky (Piomelli, U., 2001). For sensitivity analysis, runs with denser grids were also performed, with significantly improved results for both codes, but plots presented here with medium grids reveal better the weak points of the models. Besides, it is known (Piomelli, U., 2001) that grid-refined LES tends to DNS (making the SGS model of secondary importance), in contrast to RANS. It is noticed that RANS results of STAR-CD, not presented here, were also very competitive for the U^+ profile.

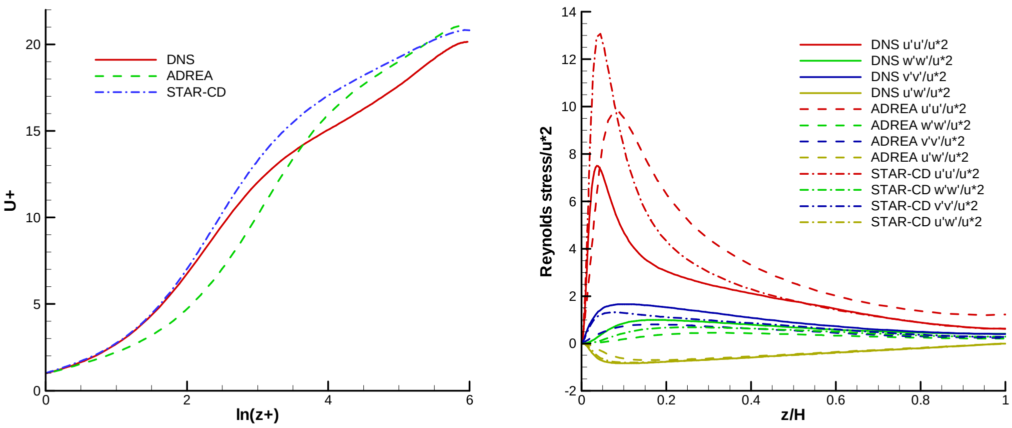

Figure 2. Velocity (left) and Reynolds stresses (right) profiles for fully developed channel flow: Comparison of ADREA-HF LES results with STAR-CD LES results and reference DNS data from Moser, R. D. *et al.* (1999). u^* is the friction velocity.

Concerning the Reynolds stresses, again the general shape of the curves is captured from LES. It is noticed that only the resolved components are provided for LES, something that partly explains the underprediction of most of the Reynolds stresses' strength. The main component $u'u'$ is clearly overpredicted though, especially from STAR-CD. On the other hand at ADREA-HF the maximum stresses values are at higher distances from the wall than at the DNS. In general, ADREA-HF proved competitive in this difficult test, even if there is room for improvement.

Street canyon

Figure 3 shows the vertical profiles of velocities and their fluctuations inside the street canyon.

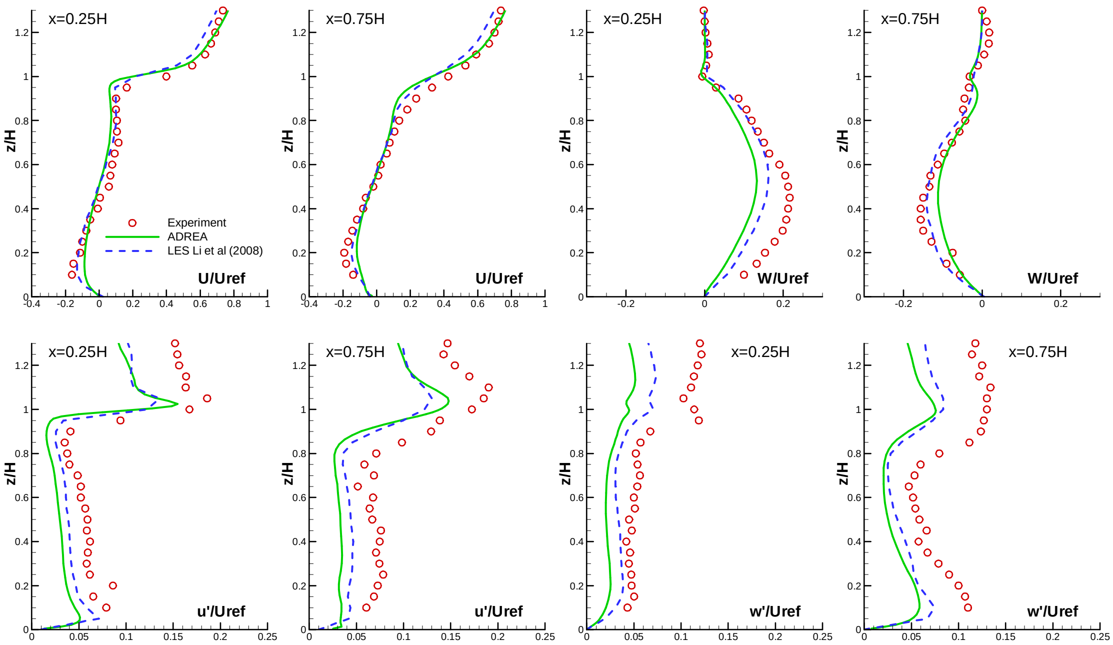

Figure 3. Velocity (top) and Reynolds stresses (bottom) profiles for street canyon flow: Comparison of ADREA-HF LES results with Li *et al.* (2008) LES results and experimental data from Li *et al.* (2008b). *x* is the distance from the upwind building.

ADREA-HF LES is evaluated against experimental data and the fine-grid LES of Li, X. X. *et al.* (2008). Despite the much coarser grid used in our simulation, ADREA-HF performs very close to the other LES, capturing all the important features of the flow and providing profiles with very similar shape to the experimental and fine-LES ones. It is clear though that both LESs and especially the one of ADREA-HF, underestimate the main vortex strength and the turbulence intensities. It should be noticed however, that the non-dimensionalization with U_{ref} might be a source of uncertainty in this case. Also three-dimensional phenomena that might be present in the experiment were absent in the infinite street canyons of the LES simulations. Finally, vortex generators used at the experiment can partly explain the higher turbulence intensities and the stronger vortex observed in Figure 3.

For sensitivity analysis, ADREA-HF runs with higher domain, uniform grid, more grid points and use of simple wall functions in a high-Reynolds case were also performed. From those simulations, the well known in the literature fact that the use of wall functions (or of a similar technique, see Piomelli, U., 2001 for an introduction) is unavoidable in real, high Reynolds urban flow cases was made clear. Indeed, the calculation time for LES is proportional to $Re^{2.4}$ close to the wall

($Re^{2.75}$ for DNS) (Piomelli, U., 2001), while away from the wall it is proportional only to $Re^{0.5}$. Also, the use of wall functions does not deteriorate the quality of the results in many cases. For example, Li, X. X. *et al.* (2008) also performed an LES simulation with use of wall functions, with results very close to their well-resolved LES presented here. Before ending this paragraph, it should be mentioned that in real urban flows, a big difficulty will also be the determination of the (turbulence-compatible) inlet boundary conditions, in case cyclic boundary condition cannot be used.

CONCLUSIONS

The incorporation of the LES methodology into the ADREA-HF code was successful and the code proved capable of performing competitive LES calculations. There is though room for improvement and refinement of the LES, like the incorporation of a wall-function-type methodology to rapidly compute the near wall region and the testing of more SGS models. From the user's point of view, the orders-of-magnitude more expensive LES calculation compared to RANS should be stressed, making LES an attractive choice mainly only for cases where RANS fails, like unsteady three-dimensional boundary layers and separated flows (Piomelli, U., 2001). Finally the difficulty in providing the appropriate boundary conditions and the relevant sensitivity of LES to them might also be an inconvenience for the potential LES user.

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