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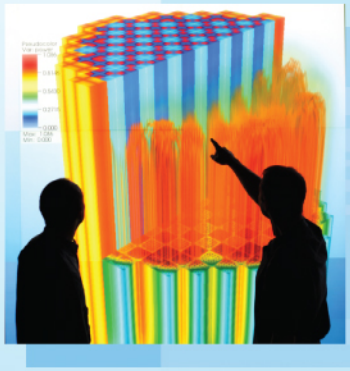

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Solution Verification Applied to TransAT Large Eddy Simulations for Smooth Wall Channel Flow With Periodic Boundary Conditions, Revision 1

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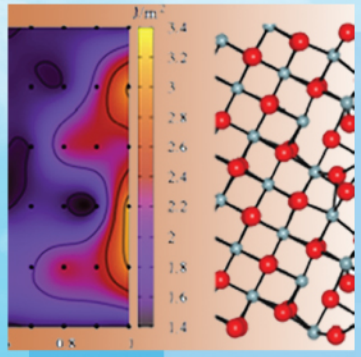

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Solution Verification Applied to TransAT Large Eddy Simulations for Smooth Wall Channel Flow With Periodic Boundary Conditions

REVISION 1

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1 Introduction

This report summarizes the solution verification procedure for smooth wall channel flow simulations conducted at MIT using the code TransAT©. The analysis implements the solution verification procedure recently proposed by the VUQ group at SANDIA [1]. The procedure had been previously applied to two cases: laminar smooth channel flow and turbulent smooth channel flow using the Large Eddy Simulation (LES) approach with the WALE [2] subgrid scale model (SGS). For the laminar channel flow case the convergence rate was found to be in very good agreement with the theoretical one (Appendix I). For the turbulent channel flow case the solution convergence was not in agreement with the theoretical convergence rate of the discretization scheme used (Appendix II). This discrepancy was attributed to the insufficient grid resolution and/or to the discretization size interfering with the LES filtering procedure.

In the present report, a study of the turbulent smooth channel flow using LES is conducted again, using finer spatial discretization. The main objective of the study is to determine whether the inadequate discretization in our previous simulations had been the reason for the divergence of the solution in our previous study. Indeed, the current study demonstrates that employing finer grids yields a rate of convergence close to the theoretical one for this class of problems. In the present study, the MPI version of the code was used since the computational cost of the simulations made running on multiple processors (HPC on jaguar) imperative. Also, for further evaluation of the quality of our LES, a Direct Numerical Simulation of the same test case has been conducted.

Following the step-by-step workflow proposed by the VUQ Group, short descriptions of the code, the numerical algorithm and the employed models are given first (Section 2), followed by a discussion of the numerical accuracy and the stability properties of the approach adopted (Section 3). In Section 4, the convergence rate evaluation procedure is described. In Section 5, the turbulent channel flow case setup is presented, the quality of our LES simulations is determined and the rate of convergence is examined. Finally, in Section 6, we give some concluding remarks and conduct an overall assessment of the analysis.

2 TransAT description

The CFD/CMFD code TransAT© developed at ASCOMP Switzerland is a multi-scale, multi-physics, conservative finite-volume code based on solving the single- and multi-fluid Navier-Stokes equations. TransAT exists in two versions: Single Block (TransAT-SB) and Multi-block (TransAT-MB). While TransAT-SB is parallelized using the OpenMP-Protocol on PC's and laptops, TransAT-MB uses MPI and domain decomposition methods to run on non-shared memory supercomputer clusters. The code uses structured multi-block meshes, with the grids having two layers of ghost cells where information from neighboring blocks is received. An MPI parallel based algorithm is used in connection with multi-blocking. The grid arrangement is collocated and can thus handle curvilinear skewed grids more easily. The solver is pressure based (Projection Type), corrected using the Karki-Patankar technique for low-Mach number compressible flows. High-order time marching and convection schemes can be employed; up to 3rd order Monotone schemes in space and 5th order in time. Turbulent flows can be treated in three ways: RANS statistical models, Scale Resolving Approaches like LES and its DES and VLES variants,

and pure DNS/ LES (and DNS) is built within the explicit version of the code, with its proper routines for pressure coupling, boundary conditions, diffusive fluxes and near-wall stress integration. TransAT uses high-order schemes for convection and diffusion processes in the linearized, discretized transport equations.

Briefly, the schemes employed for convection in all equations are: HLPA (2nd order), CENTRAL (2nd order), QUICK (3rd order), SOUCUP (2nd order), HYBRID & UPWIND (1st order), TVD-based Schemes (2nd order). The schemes employed for time marching are the following: EULER (1st and 2nd order), TLFI (2nd order), Runge-Kutta (2nd to 5th order). The schemes employed for pressure-velocity coupling are: SIP, GMRES, GMG & AMG, augmented using the parallel PETSc solver library. For large-scale problems, TransAT is parallelized using Message Passing Interface (MPI).

For the simulations discussed here the Multi-Block version of the code was used (TransATMB_par-2.1.1.16) running on High Performance Supercomputing Facility 'Jaguar'. For all our the turbulent test cases Large Eddy Simulations were performed, where the larger three-dimensional unsteady turbulent motions are directly represented, whereas the effect of the smaller scale motions is modeled as a subgrid scale viscosity.

3 Numerical Method Summary

All our simulations are carried out using the 2nd order accuracy Central Difference scheme for the discretization of the convective fluxes, and the 2nd order accurate HLPA scheme for density. An explicit 3rd order Runge-Kutta scheme is used for time integration. The timestep is bounded by a stability criterion (CFL) fixed between 0.1 and 0.3 to guarantee stability of the simulations. The flow is incompressible and the simulations are conducted in three dimensions. No wall functions are used for the near wall region solution. For the pressure-velocity coupling the SIMPLE algorithm is used. The SIP preconditioned GMRES is used for the pressure solver. The simulations run on multiple cores on the supercomputer Jaguar using MPI. The specifics of each simulation are described in Section 5.

4 Convergence rate

The methodology employed here follows the procedure proposed by the VUQ Group from SANDIA [1]. We employ indeed three solutions g^k obtained for different grid resolutions, for $k= vc, c, f$, where k is defined as 'very coarse (k=*vc*)', 'coarse (k=*c*)' and 'fine (k=*f*)'. Equivalently, the mesh for each simulation is denoted as $\bar{\Delta}$.

The actual order of accuracy of the solution is given by:

$$\alpha = -\left[\log\left\|g^f - g^c\right\| - \log\left|g^c - g^{vc}\right\|\right] / \log\sigma \qquad where \quad \sigma \equiv \bar{\Delta}^c / \bar{\Delta}^f \tag{1}$$

Additionally, the ratio of the signed error in the solution from one mesh refinement to the next can be used as a means to characterize the solution convergence order. That is:

$$R = (g^f - g^c)/(g^c - g^{vc})$$

$$\begin{aligned} &if\ \ R < 1\ then\ monotonic\ convergence \\ &else\ if\ \ R > 1\ then\ monotonic\ divergence \\ &else\ if\ \ R < -1\ then\ oscillatory\ \ divergence \\ &else\ \ (-1 < R < 0)\ then\ oscillatory\ \ convergence \end{aligned} \tag{2}$$

5 Turbulent channel flow using Large Eddy Simulation (LES)

5.1 Code input parameters and problem definition

5.1.1 Geometry, Boundary and Initial conditions

Turbulent flow in a channel with smooth walls is considered. The fully-developed turbulent solution is homogeneous in the streamwise and spanwise directions, which implies using periodic boundary conditions in these two directions is an accurate assumption. The computational domain size was chosen such that it includes the largest eddies of turbulence in the flow and these eddies are not correlated. The flow is along the x-direction; the y is the wall-normal direction with no-slip conditions applied to it.
The simulation domain consists of a Cartesian box of dimensions Lx = 2πh, Ly = 2h, and Lz =πh, where h is the half-height of the channel which is used as the characteristic lengthscale.
Initial turbulent flow conditions are generated based on the homogenous flow properties which implies that the velocity fluctuations are isotropic and could be determined based on the shear velocity, i.e. u' =v' = w' = variance of u_τ (friction velocity).

5.1.2 Setup

The desired value of the friction Reynolds number (Re_τ), which here is taken to be 400 is obtained by fixing the density and the viscosity values ($\rho = 1Kg/m^3$ and $\mu = \mathrm{Re}_\tau^{-1}$), and by adding a unity pressure gradient source term in the 'x-momentum' equation. This implies that the bulk velocity of the fluid has to adjust in order to maintain the pressure forcing term.
Statistics are computed from solution samples, once statistically ergodic conditions have been reached for all the cases. Space averaging is performed in the streamwise and spanwise directions throughout the whole domain. The time-averaging interval is one timestep.
For the LES of turbulent channel flow the subgrid scale model used was the WALE model. From a previous study on the same topic both the Smagorinsky and the Dynamic [3] model were found to perform worse than the WALE [2] model for this specific case. This is why, in this study we chose to use only the WALE model.

5.2 Sequence of discretization and relevant parameters

Three numerical grids have been used to test the convergence behavior of our simulations. The grid in the near-wall region is finer than in the rest of the domain. The grid becomes coarser towards the centerline of the channel and the refinement ratio is 1.15 in all our simulations. A typical grid can be seen in Figure 1.

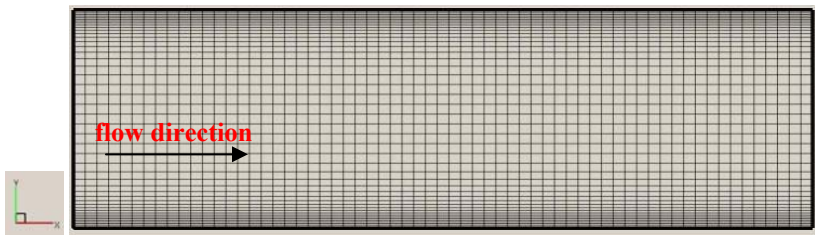

Figure 1. Typical grid used for our simulations.

The refinement ratio between two consecutive grids is $\sqrt{2}$ ($\sigma = \sqrt{2}$) applied everywhere in the domain. The same rule applies to both the number of processors used and to the total number of cells for each simulation (applied to all three dimensions, so it is $2\sqrt{2}$). The details are shown in Table 1. The grid size is expressed in y^+ units.

Table 1. LES simulation resolution

$\mathrm{Re}_\tau = 400$	Number of nodes			Resolution				Number of processors	Approx. total number of cells
	x	y	z	Δx^+	$\Delta y^+_{\min}$	$\Delta y^+_{\max}$	Δz^+		
Grid 1 'vc'	91	68	68	27.74	2.56	16.00	18.48	24	**0.4 M**
Grid 2 'c'	128	96	96	19.61	1.81	11.31	13.07	60	**1.2 M**
Grid 3 'f'	181	136	136	13.87	1.28	8.00	9.24	168	**3.3 M**

The determination of the characteristic length scale ($\bar{\Delta}$) for every simulation was done by using the following:

$$\bar{\Delta} = \left[\frac{1}{N} \sum_{i=1}^{N} \left(\Delta V_i \right) \right]^{\frac{1}{3}} \tag{3}$$

where ΔV_i is the cell volume and N is the total number of cells used in our computations.

5.3 Simulation accuracy and quality assessment

The SGS model in LES commonly employs information from the smallest resolved scales as the basis for modeling the stresses generated by the unresolved turbulent eddies. Consequently, it is imperative that the resolved lengthscales are captured accurately by the numerical scheme. This, in turn, requires that the numerical error of the scheme is sufficiently small and hence, high order numerical schemes are necessary. The grid resolution affects not only the numerical discretization error but also the subgrid scale (SGS) model contribution in terms of energy. Further, these quantities are coupled, thereby adding to the complexity of the assessment [4]. In the present report, not only do we conduct a convergence rate analysis but we also assess the quality and the accuracy of our LES simulations using the index proposed by Celik et al. [5] as well as by comparison to a DNS study respectively.

5.3.1 Accuracy

To assess the accuracy of all our LES simulations we compare some representative quantities with those of a Direct Numerical Simulation conducted using the same executable, ran on the same machine. The details of the DNS simulation are shown in Table 2.

Table 2. DNS simulation resolution and simulation parameters

$\mathrm{Re}_\tau = 400$	**Number of nodes**			**Resolution**				**Number of processors**	**Approx. total number of cells**
	x	y	z	Δx^+	$\Delta y^+_{\min}$	$\Delta y^+_{\max}$	Δz^+		
Grid 2	256	192	192	9.81	0.91	5.65	6.54	480	**9.3 M**

In Figure 2, both the mean velocity profile and the stress profiles are shown for all our LES simulations in comparison with the DNS simulation. A reference DNS simulation [6] of the same case is also plotted for additional validation. As it can be seen, the LES show very good comparison with the DNS and the agreement with the DNS solution is increasing with increasing grid refinement.

5.3.2 Quality

To assess the quality of all our Large Eddy simulations we use the total turbulent kinetic energy from the DNS k^{DNS} and the resolved turbulent kinetic energy from the LES k^{res}. The local turbulent kinetic energy in both cases has been computed as:

$$k = \frac{1}{2}\sqrt{\overline{\left(u'\right)^2} + \overline{\left(\overline{v}'\right)^2} + \overline{\left(\overline{w}'\right)^2}} \tag{4}$$

The overall turbulent kinetic energy has been computed as the integral of (4) in the entire computational domain. The index giving the quality of the LES is given by the following equation taken from Celik et al. [5]:

$$IQ_DNS = 1 - \frac{\left|k^{DNS} - k^{res}\right|}{k^{DNS}} \tag{5}$$

The results for all three LES are shown in Table 3. The quality of the LES is very high as the resolved turbulent kinetic energy is more than 94% of the kinetic energy computed in a DNS simulation.

Table 3. LES quality assessment using the IQ_DNS

LES for $\mathrm{Re}_\tau = 400$	**Grid 1**	**Grid 2**	**Grid 3**
IQ_DNS	0.941	0.957	0.967

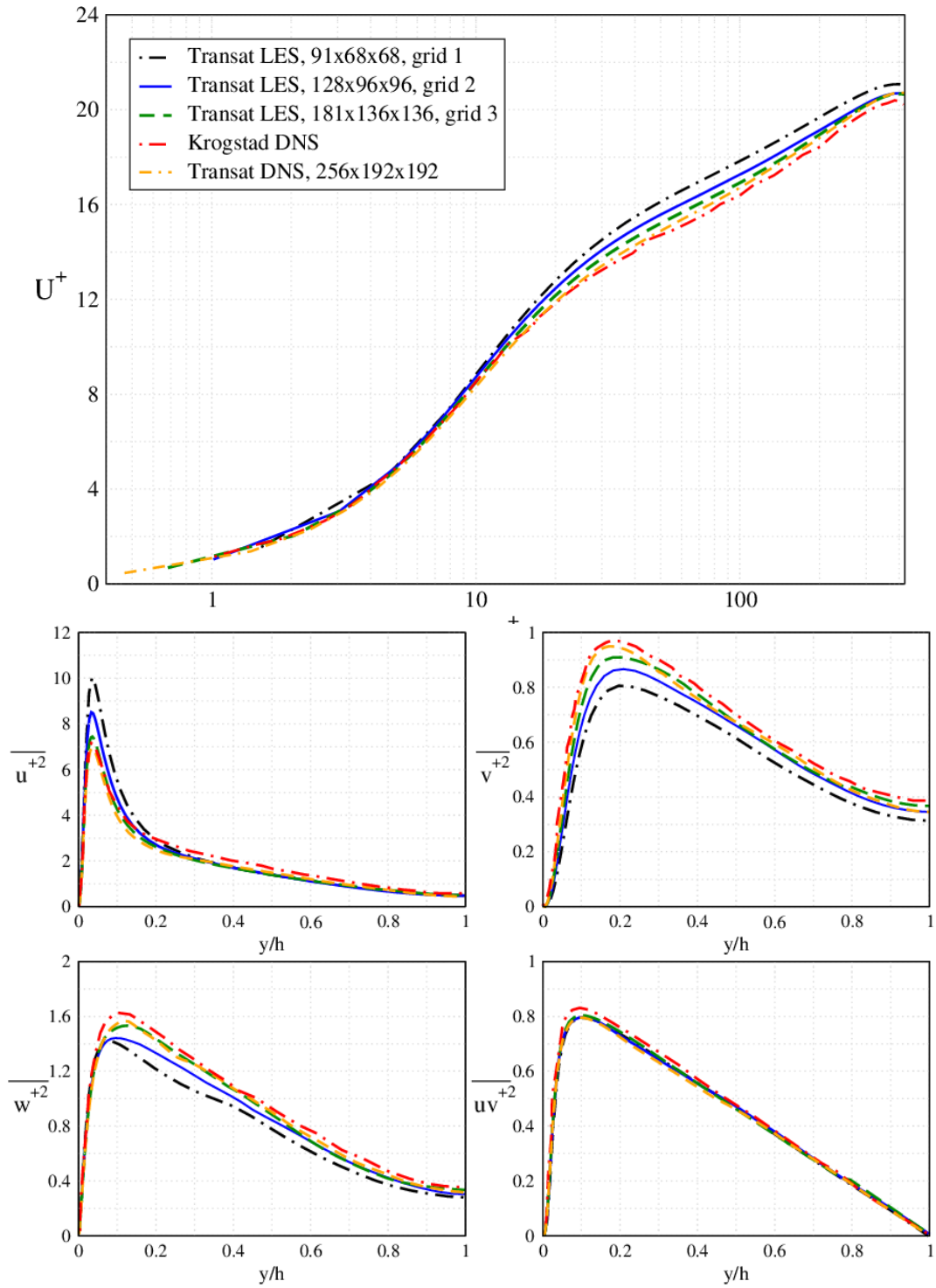

Figure 2. Comparative plots of mean velocity profile, streamwise, wall-normal, spanwise and shear stresses for all three LES simulation with Transat DNS and Krogstad et al. (2005) [6] DNS of the same case for $\mathrm{Re}_\tau = 400$**.**

5.4 Convergence rate

5.4.1 Choice of metrics

For the convergence analysis both integral quantities and field variables are chosen in order to have a complete image of the convergence behavior. More specifically, the Figures of Merit chosen are 1) the bulk velocity (U_{bulk}), 2) the space and time averaged centerline streamwise velocity of a point right at the center of the channel (πh, h, $\pi h/2$), and 3) the turbulent kinetic energy of the entire domain (integral quantity). Additionally, the integral of the time and space averaged Subgrid Scale Viscosity (Eddy Viscosity) has also been used here in order to support the analysis. The value of the actual convergence rate α based on the different Figures of Merit is presented in Table 4.

When using the bulk velocity as the Figure of Merit, in all three simulations, an averaging procedure has been applied to a time period defined by two consecutive minima or maxima of the bulk velocity value in time.

Table 4. Convergence rate α

α (U_{bulk})	R (U_{bulk})	α (U_{cent}^+)	R (U_{cent}^+)	α (k^+)	R (k^+)	α (sgvis)	R (sgvis)
4.08	0.24	2.44	0.42	2.9	0.35	1.14	0.67

There is a large overestimation of the convergence rate for U_{bulk}; fairly good agreement with theoretical convergence rate (2) for U_{cent}^+ and k^+, and an underestimation for sgvis. The solution exhibits a monotonic convergence behavior in all cases.

6 Overall assessment

A convergence rate analysis has been performed using the code TransAT. Due to problems in the convergence in previous LES simulations, not only was there a finer discretization approach applied but the authors also evaluated the quality of the LES simulations and showed good accuracy when comparing with the DNS of the same test case. The convergence rate of the spatial discretization scheme was found to be in reasonable agreement with or higher than 2nd order which is the theoretical convergence rate.

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[2] Nicoud, F. and Ducros, F., 'Subgrid-scale Modeling Based on the Square of the Velocity Gradient Tensor', Flow, Turbulence and Combustion, 62, pp. 183-200, 1999.

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[4] Speziale, C. G., 'Turbulence Modeling for Time-Dependent RANS and VLES', AIAA J., 36(2), pp. 173-184, 1998

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[6] Krogstad, P.-Å, Andersson, H. I., Bakken, O. M., Ashrafian, A., 'Comparison Between Rough- and Smooth-Wall Turbulent Boundary Layers., J. Fluid Mech, 245, pp. 599-617, 1992

Appendix I. Laminar smooth channel flow case

Setup

The desired value of the bulk Reynolds number (Re), which here is taken to be 1000 is obtained by fixing the density, the viscosity and the bulk velocity ($\rho = 1\ Kg/m^3, \mu = U_{bulk} \cdot \mathrm{Re}^{-1}, U_{bulk} = 10\ m/s$). This implies that the friction velocity of the fluid has to adjust in order to maintain the prescribed bulk velocity. The simulation is steady state. A uniform grid is used (details are described below).

Sequence of discretization and relevant parameters

Four numerical grids have been used to test the accuracy of our simulations. All spatial discretizations were uniform throughout the entire domain. For each subsequent discretization, the grid has been refined by a factor of 1.5 (σ =1.5). The details are shown in Table I.1 and a typical grid can be seen in Figure I.1.

Table I.1. Grid characteristics

	Grid (N_x,N_y,N_z)	Discretization size (m) $\bar{\Delta}$
Very Very coarse (vvc)	32x11x16	0.18209
Very coarse (vc)	48x16x24	0.12896
Coarse (c)	72x24x36	0.08588
Fine (f)	108x36x54	0.05722

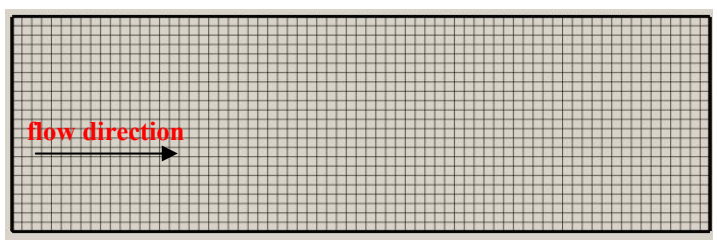

Figure I.1. Typical grid used for our simulations. 72x24x36 example.

Choice of metrics

The metrics that are chosen for the convergence analysis are representative of the problem. One of these is the streamwise centerline velocity, which is the maximum velocity value in the entire domain and we expect it to be 3/2 of the bulk velocity. The second figure of merit is the wall shear stress τ_w, a value representative of the accuracy of the simulation since it has to be adjusted by the code throughout the simulation so that a fixed bulk velocity is maintained. All the results presented here are obtained after the shear stress value has converged to a constant value.

Discretization errors and convergence rate

The four different uniform grids from Table I.1 are used to check the convergence rate of the simulation. The theoretical convergence rate for the Central Difference Scheme used here is 2. To perform the check using equation (1), the last three and the first three discretizations shown in Table 1 are used. The results

can be seen in Table 2, for both sequences and for both figures of merit, $U_{centerline}$ and τ_w. An additional check is to estimate the solution convergence order. That can be done by using equation (2). The results are reported in Table I. 2.

Table I. 2. Convergence rate α

grid sequence	α based on $U_{centerline}$	R based on $U_{centerline}$	α based on τ_w	R based on τ_w
c-vc-vvc	1.9748	0.449	1.9749	0.449
f-c-vc	2.1333	0.421	1.896	0.463

The values of α presented in Table I.2 indicate that the actual convergence rate of our simulations is very close to the theoretical convergence rate. Also, since R<1 the solution exhibits a monotonic convergence behavior. The relevant plots can be seen in Fig. I.2 below.

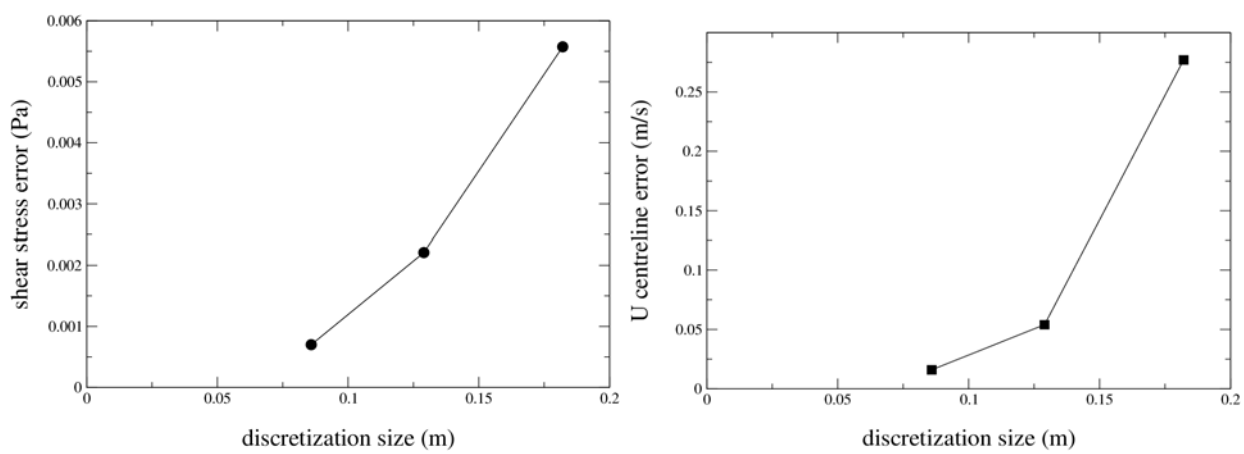

Figure I.2. Discretization error for laminar channel flow case based on the shear stress and centerline velocity figures of merit.

Appendix II. Large Eddy Simulation of turbulent smooth channel flow case (low spatial resolution simulations)

Setup

The desired value of the friction Reynolds number (Re_τ), which here is taken to be 400 is obtained by fixing the density and the viscosity ($\rho = 1Kg/m^3$ and $\mu = \mathrm{Re}_\tau^{-1}$), and by adding a unity pressure gradient source term in the 'x-momentum' equation. This implies that the bulk velocity of the fluid has to adjust in order to maintain the pressure forcing term.

Statistics are computed from 40,000 solution samples once statistically ergodic conditions have been reached for all the cases. Space averaging is performed in the streamwise and spanwise directions throughout the whole domain. The averaging interval is one timestep (collecting samples at every timestep). From a previous study on the same topic both the Smagorinsky and the Dynamic model were found to perform worse than the WALE model for this specific case. This is why, in this study we chose to use only the WALE model.

Sequence of discretization and relevant parameters

Four numerical grids have been used to test the accuracy of our simulations. The grid in the near-wall region is finer than in the rest of the domain. The grid becomes coarser towards the centerline of the channel and the refinement ratio is 1.15 in all our simulations. A typical grid can be seen in Figure II.1. The grid has been refined by a factor of $\sqrt{2}$ ($\sigma = \sqrt{2}$) everywhere in the domain. The details are shown in Table II.1.

Table II.1. Grid characteristics

	Grid (N_x,N_y,N_z)	Discretization size (m) $\bar{\Delta}$
Very Very coarse	23x17x17	0.1487
Very coarse (vc)	32x24x24	0.0989
Coarse (c)	45x34x34	0.0616
Fine (f)	64x48x48	0.0462

Only the three finest grids were taken into account in the convergence rate analysis, but the coarser one was also used to illustrate the trend of the results.

Choice of metrics

The Figures of Merit chosen here for the convergence analysis are 1) the bulk velocity (U_{bulk}), 2) the space and time averaged centerline streamwise velocity of a point right at the center of the channel (πh, h, πh/2), and 3) the streamwise normal stress profile of the same point at the center of the channel, which is representative of the turbulent kinetic energy. The time and space averaged Subgrid Scale Viscosity (Eddy Viscosity) has also been used here in order to support the analysis.

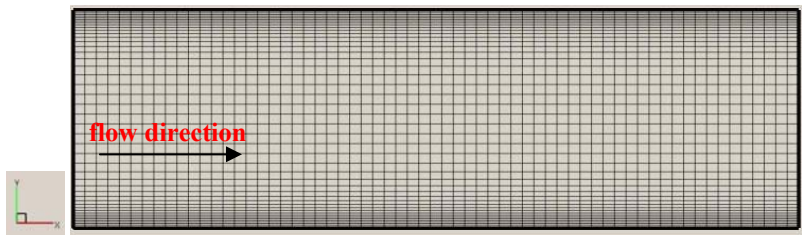

Figure II.1. Typical grid used for our simulations. 64x48x48 example

Discretization errors and convergence rate

The value of the actual convergence rate α based on the different Figures of Merit is presented in Table II. 2. If we base our analysis on the bulk velocity or on the mean streamwise centerline velocity, the behavior of the simulations appears to be diverging, instead, if we base it on the mean streamwise stress the convergence rate appears to be relatively close to the theoretical convergence rate.

Table II. 2. Convergence rate α

α based on U_{bulk}	R (U_{bulk})	α based on U^+	R (U^+)	α based on u^{+2}	R (u^{+2})
-0.817	1.327	-1.127	1.478	1.617	0.571

In Figure II. 2 and Figure II. 3 the Figures of Merit are plotted against the discretization size. Clearly, the convergence behavior does not appear to be monotonic and conclusions cannot really be made about the accuracy of these simulations. Similar behavior has been reported in the literature [8,10].

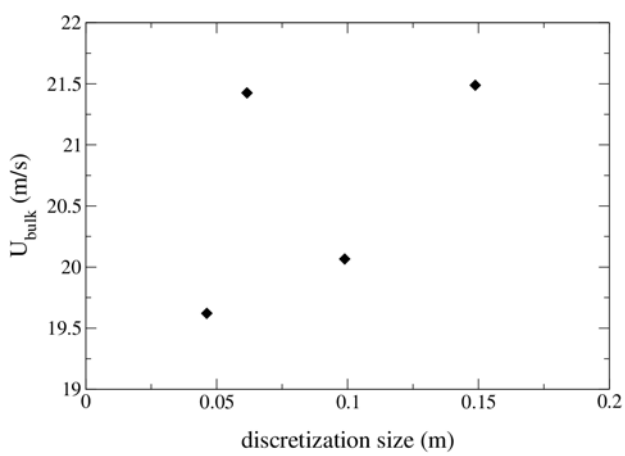

Figure II. 2. Bulk velocity (U_{bulk}) as a function of the discretization size. Although the velocity seems to follow a decreasing trend, there is one point that is far from this trend.

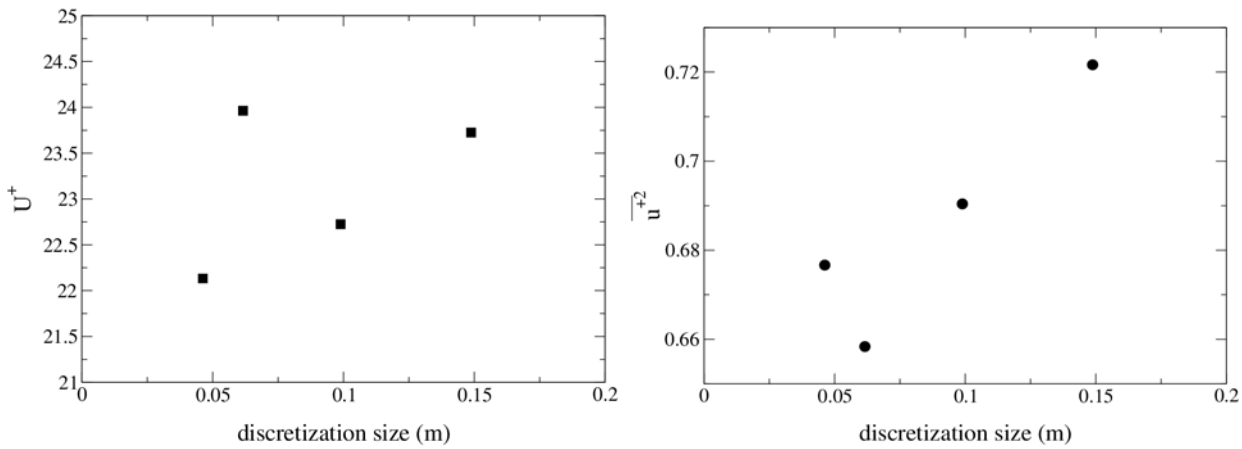

Figure II. 3. Non-dimensional profiles of the mean centerline streamwise velocity of a point at the center of the channel and the mean streamwise normal stress profile at the same point.