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V. K. Chakravarthy
Georgia Inst. of Technology, Atlanta

S. Menon
Georgia Inst. of Technology, Atlanta

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On large eddy simulation of non-homogeneous flows*

V. K. Chakravarthy ‡ & S. Menon†
School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0150

ABSTRACT

The performance of the subgrid kinetic energy equation model for a wall bounded inhomogeneous flow is evaluated and reported in this paper. Near wall behavior has eluded any kind of modeling in turbulence simulations. Most Large eddy simulations have a near DNS (direct numerical simulation) resolution in the near wall region. As a consequence, the finite difference computation of the derivatives need special attention because of the rapid stretching encountered in the near wall region. This increases the computational expense and is perhaps one of the major factors preventing LES as an affordable tool in engineering. The effect of inadequate grid resolution and unresolved viscous sublayer phenomena on the core region turbulence is studied. Such a study could provide valuable information for developing LES models that could predict turbulence away from the wall despite the errors in the near wall region or for development of simple empiricisms to account for near wall effects in a LES. It is shown in this study that the subgrid kinetic energy model shows a tendency of capturing, at least qualitatively, the near wall turbulence and could be used as a starting point for development of near wall models that could be used in conjunction with large eddy simulations.

1 Introduction

In the recent years, the dynamic evaluation procedure has greatly enhanced the performance of the large eddy simulation models (see Germano et al. [1]). This procedure is used to determine the model coefficients in large eddy simulation (LES) models by assuming that the model is valid at the grid scale and a larger resolved scale (corresponding to the test filter width). Given the fact that the spectrum at the test filter scale corresponds to the form assumed in deriving the LES model, this technique can greatly extend the use of LES in modeling of complex flows. In this study, we focus on the issues concerning LES of wall bounded turbulent flows. Temporally evolving pressure driven flow in a square duct at two different Reynolds numbers is considered. Each of these flows have secondary flow patterns that present a great difficulty in terms of subgrid modeling. The performance of the dynamic LES model is evaluated in these complex flows.

The flow in a square duct is an ideal choice for the present study because it has two inhomogeneous directions and two mutually perpendicular boundary layers. The interaction between these two layers gives rise to secondary flow patterns in the cross plane. The flow normal to the streamwise direction is directed away from the center towards the corners of the duct where it gets turned around creating recirculatory patterns. These patterns have been the root cause of the difficulty in terms of turbulence modeling. Speziale [2] has shown that these patterns are related to the fact the normal Reynolds stresses are unequal and hence the much used $K-\epsilon$ model in Reynolds averaged approach fails. There have been attempts to model this flow field using non-linear $K-\epsilon$ model [3], but the results are not fully satisfactory. A large eddy simulations, given that it has in it, less empiricisms in terms of modeling may be a better tool for this purpose. The secondary flow patterns in this flow have been studied in detail by Gavrilakis [4] and Reichert et al.[5] using high resolution DNS. Their results provide a basis

† Associate Professor, Senior Member, AIAA.

‡ Graduate Research Assistant.

against which the results of the present LES could be compared.

The LES models are usually derived with an assumption that the subgrid scales are isotropic. This is very unlikely in case of many inhomogeneous flows (at Reynolds numbers encountered in engineering applications) resolved at a grid size limited by the present day computational resources. In using LES to model such flows, it is assumed that the weak homogeneity that exists in the subgrid scales does not significantly affect the evolution of the large scales in the flow. Furthermore, the flow near a solid wall does not follow the phenomenology applied in modeling fully developed turbulence. The accurate prediction of near-wall behavior without resolving all the relevant scales is beyond the present stage of modeling in turbulence. Very fine grids are still needed to resolve the near wall phenomena, thus, requiring very high grid stretching. Special finite difference approximations need to be constructed in these regions and usually these are lower in order and increase the computational cost enormously. This may not be affordable or practical for use in LES. In the present study, the impact of using coarse grids near walls on LES is studied. The eventual goal is to ensure that the errors in near wall region do not diffuse into the interior of the flow field and destroy the overall accuracy of the prediction. The near wall behavior, however, cannot be accurate but in this study, LES is mostly targeted towards modeling combustion and mixing which seldom occur in the vicinity of the walls. If one were to use LES for predictions that depend heavily on near wall behavior like the fluid dynamic drag, there is no choice but to cluster the grid in the wall region.

The governing equations and numerical methods used are explained in the next section. Section 3 details the model used in the simulation along with the dynamic evaluation procedure. The results from the simulations, conclusions and suggestions for future research can be found in the last section.

2 Governing equations

The Navier-Stokes equations, on convolution with a spatial filter, reduce to the following set of LES equations.

$$\frac{\partial \overline{U}_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\mathrm{d}\overline{U}_i}{\mathrm{d}t} = -\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{U}_i}{\partial x_k \partial x_k} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

where the overbar indicates a filtered variable, $\tau_{ij} = (\overline{U_i}\ \overline{U_j} - \overline{U_i U_j})$ is the subgrid stress. For a closed set of equations , one needs to approximate the subgrid stresses using a model. The velocity variations in the scales below the characteristic filter width Δ are unresolved in a LES. Due to the nonlinear nature of the Navier-Stokes equations, these small scale fluctuations effect the large scale motions. This effect comes from the subgrid stress, which in the present study is approximated as $\tau_{ij} = -\frac{2}{3}K\delta_{ij} + 2\nu_t \overline{S_{ij}}$, where $\overline{S_{ij}} = \frac{1}{2}\left[\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i}\right]$ is the resolved strain tensor, ν_t is subgrid eddy viscosity (to be defined later) and $K = -\frac{1}{2}(\overline{U_i}\ \overline{U_i} - \overline{U_i U_i})$ is the subgrid kinetic energy. Filtered variables are also called supergrid variables because they carry information about a variables at all length scales above the filter width (set equal to the grid spacing here, although not necessary). The model equations for the subgrid kinetic energy and the eddy viscosity are presented in the next section.

The equations are discretized on a non-staggered grid (with spacing corresponding to the characteristic filter width Δ) and numerically integrated using a two step semi-implicit fractional step method. In this method, all of the primitive variables are defined at the grid points. The well known checker board type oscillations occur in velocity field due to velocity-pressure decoupling when one uses central finite difference schemes for approximating the spatial derivatives. Use of QUICK scheme for calculation of velocity gradients that arise in the source term of the elliptic equation for pressure is found to effectively couple the velocity and pressure fields, thus, removing these oscillations [6]. The convective terms are computed using a upwind biased finite difference approximations (third-order in wall normal and fifth-order in streamwise directions) while the viscous terms are computed using a fourth-order central difference approximation. The Poisson equation is solved numerically using a second-order accurate elliptic solver that uses a four-level multigrid scheme to converge the solution. The finite difference equations are integrated in time using a second-order scheme.

3 LES Model

A K-equation model with dynamic evaluation of the model coefficients based on the Germano's filtering approach is used as a LES model. First proposed by Schumann, the K-equation model been shown to be very useful especially in LES of reacting flows (see Weeratunga and Menon [7]). The advantage of this model is that it solves a single scalar equation for the subgrid kinetic energy which characterizes the velocity scale of subgrid turbulence. This velocity scale along with the length scale (grid spacing or the filter width) provides a subgrid timescale representing the non-equilibrium relaxation of the subgrid scales. This is one step forward (in the direction of developing non-equilibrium models) than the equilibrium models(algebraic or the zero equation models), wherein the production and dissipation of the subgrid kinetic energy are assumed to balance instantaneously.

Menon and Kim [8] suggested a dynamic modeling approach using the K-equation model. The amount of subgrid kinetic energy in the subgrid scales gives the extent of unresolved scales (energy content as well as the range). Given the fact that the modeling of resolved scales is yet far from accurate, the subgrid kinetic energy can be looked upon as an error estimator in a LES. On the other hand, LES using algebraic models can give no information in this regard. It is imperative while using algebraic models that the grid scale cut off lie in the dissipative end of the inertial range of scales (because of the assumption that subgrid production equals dissipation). One has to rely on experimental results or grid independence tests (sometimes involving usage of near DNS resolution grids for the purpose) for validation. On the other hand, in the one equation model the grid scale cut-off could be at a larger scale (in the inertial range), allowing coarse grid large eddy simulations.

Only an outline of the present model is provided here, since a more comprehensive description, including the implementation issues, can be found in Ref.8. The eddy viscosity and subgrid dissipation in physical space, for a characteristic filter width Δ, are given as follows.

$$\nu_t = C_\nu K^{\frac{1}{2}} \Delta, \tag{3}$$

$$\epsilon^{sgs} = C_\epsilon \frac{K^{\frac{3}{2}}}{\Delta} \tag{4}$$

These expressions are same as the expressions obtained if one uses dimensional arguments considering the subgrid kinetic energy and filter width as the relevant parameters for determining the subgrid eddy viscosity. The assumptions made in arriving at these expressions from analytical arguments in turbulence and their validity are discussed to some extent in ref.9.

For the transport term, a gradient diffusion model based on eddy diffusivity model (with unit eddy Prandtl number) has been proposed and studied by Menon and Kim. This approximation was found to adequately model the transport terms. Hence this is used in a similar form in this study. The dynamic equation for K can now be written as:

$$\frac{\partial K}{\partial t} + \overline{U_j} \frac{\partial K}{\partial x_j} = \tau_{ij} \frac{\partial \overline{U_i}}{\partial x_j} - \epsilon^{sgs} + \frac{\partial}{\partial x_j} \left[\nu_t \frac{\partial K}{\partial x_j} \right] \tag{5}$$

C_ν and C_ϵ are the model constants that need to be specified. These constants, however, are not universal and differ with flow fields in general. This suggests that these constants also depend on the local (supergrid) structure of the flow field. It is, then appropriate to refer to them as coefficients rather than constants. A dynamic approach is applied here to evaluate these coefficients. This procedure acts as an online calibration method thus removing the arbitrariness in prescribing these coefficients. The approach is based on the concept of subgrid stress similarity supported by experiments in jets (Liu et al. [10]). In this approach, a test filter(similar to the LES filter) of characteristic width 2Δ is defined and the corresponding filtered velocity field is denoted by $\widetilde{U_i}$. This new velocity field is obtained by convolution of the LES filtered velocity with the test filter. The subgrid stress corresponding to the scales in between the grid filter width and the test filter width can be written as [8]:

$$t_{ij} = \widetilde{\overline{U_i}\ \overline{U_j}} - \widetilde{\overline{U_i}}\ \widetilde{\overline{U_j}} \tag{6}$$

and the corresponding dissipation is defined as

$$e = (\nu + \nu_t) \left[\frac{\partial \widetilde{\overline{U_i}}}{\partial x_j} \frac{\partial \widetilde{\overline{U_i}}}{\partial x_j} - \frac{\partial \widetilde{\overline{U_i}}}{\partial x_j} \frac{\partial \widetilde{\overline{U_i}}}{\partial x_j} \right] \tag{7}$$

Assuming stress similarity and the present model to be valid for length scales between Δ and 2Δ (which imposes a further restriction that the test filter width is also in the inertial range of length scales), t_{ij} and e can be written as follows.

$$t_{ij} = -\frac{2}{3}\widetilde{K}\delta_{ij} + 2\widetilde{\nu_t}\widetilde{\overline{S_{ij}}} \tag{8}$$

and

$$e = C_\epsilon \frac{\widetilde{K}^{\frac{3}{2}}}{2\Delta}, \tag{9}$$

where $\widetilde{K} = -\frac{1}{2}t_{ii}$ and $\widetilde{\nu_t}$ is the eddy viscosity corresponding to the test filter of width 2Δ and is given by $C_\nu \widetilde{K}^{\frac{1}{2}}(2\Delta)$. From eq.(14), the value of C_ϵ can be evaluated. There are, however, six equations represented by eq.(8) using which C_ν could be evaluated. This is a over-determined system of equations and in the present formulation, is solved using least-squares technique. These coefficients are then used for evaluation of eddy viscosity and to advance the dynamic equation for K in time, thus achieving complete closure.

In the past studies, the spatial variation of the model coefficients evaluated using many of the dynamic approaches in the past, was found to be oscillatory and susceptible to numerical instabilities. Various methods like filtering, spatial averaging were used to remove this oscillatory behavior. The present dynamic evaluation procedure is, however, completely localized and does not lead to any instabilities in integration. The present model, hence, is a considerable improvement over the existing LES models, as shown by Menon and Kim [8].

4 Results and discussion

The turbulent flow in a square duct is simulated at two different Reynolds numbers. The flow in this geometry is strongly dependent on the interaction (discussed earlier) between the primary and the secondary flows (strain rates). This interaction was found to cause fairly strong dependence of turbulence on the Reynolds number as compared to flows with unidirectional mean shear (channel flow, Couette flow etc.). Most modeling approaches using Reynolds averaged Navier-Stokes equations rely on phenemenology of high Reynolds number asymptotics and have only a weak incorporation of Reynolds number effects. LES may be better suited for these type of flows.

Flow at a Reynolds number of 10000 (corresponding to a Reynolds number of 600 based on friction velocity and duct width) was simulated as a test case on a 65x49x49 grid with hyperbolic tangent stretching rate in the wall normal directions. The clustering of the grid at the walls is found to resolve the wall layer adequately. Owing to rapid stretching, finite difference approximations are computed using stretching dependent stencils in these directions. It is acknowledged that the effects of very non-uniform filter on LES have been ignored in this simulation. This case was chosen because of the availability of reliable DNS data at this Reynolds number (Huser and Biringen [11]).

The near wall variation of the turbulence intensities at the mid-section, normalized by local skin friction velocity is shown in fig.1(a-c) along with data from channel flow DNS (Kim and Moin[12]) and square duct DNS (Huser and Biringen [11]). The viscous sublayer turbulence is found to fairly similar in all three cases indicating a universal (but Reynolds number dependent) nature. It is well known that turbulence intensity near the wall grows with Reynolds number and this fact is reflected in the figures. The data from channel flow DNS is found to be higher because of a slightly higher Reynolds number (13200). The stream-wise turbulence intensity is overpredicted by the present LES as compared to DNS because of the coarse resolution in the stream-wise direction. Rai and Moin[13] infer that use of upwind biased scheme in an under resolved simulation tends to overpredict turbulence intensity in the direction of inadequate resolution. This fact is further confirmed by Huser and Biringen [11]. Yet it is still better to use a higher order upwind biased scheme as opposed to central or spectral schemes (though less dissipative) in order to minimize aliasing errors (see Rai and Moin[13]).

An LES is conducted with same conditions as in the previous case but with a 65x33x33 grid which is algebraically stretched out in the wall normal directions. The grid spacing in the wall normal direction near the wall is close to 10 nondimensional wall units. Considerable amount of the kinetic energy is produced in the close vicinity of the wall and it is very unlikely that this could be captured using this grid. The intent here, is to study the effect of this inadequacy on the core region turbulence. Shown in fig.2(a,b) are respectively, the variation of u'^2 and subgrid kinetic energy along the wall bisector along with corresponding values from DNS. As can be seen u'^2 is largely underpredicted (despite low axial resolution) especially in the wall region. The peak in u'^2 is shifted away from the wall. This was noticed earlier by Menon and Chakravarthy [14] in turbulent Couette flow simulated on a very coarse grid. In the present flow, it was noticed however, that the kinetic energy (resolved and subgrid) seems to be predicted with fair amount of accuracy. This perhaps may be due to the fact that the Couette flow is a wall driven flow as against the square duct (which is pressure driven) thus making the wall layer phenomena more important.

Figure 2b shows the variation of normalized kinetic energy (both resolved and the subgrid) in comparison to DNS. The total kinetic energy prediction seems satisfactory with small differences in the core region. While this may be an error in the simulation, it could also be due to the difference in axial length between the two simulations. However, the point to be noted here is that the subgrid kinetic energy is very high in this simulation. In the near wall region, the subgrid kinetic energy peaks close to where the peak in DNS is observed. While this is encouraging, as stated earlier, high subgrid kinetic energy indicates high uncertainity in the validity of the results.

It can be concluded from this study that in a LES with coarse wall layer resolution, the near wall turbulence cannot be captured with in the range of resolved scales. The phenomenology on which the subgrid kinetic energy is based, fails in this region. However, the kinetic energy does tend to peak in the near wall region as if to capture the unresolved turbulence, but, this could also be an indication of high modeling uncertainity.

A Re = 5000 simulation was then conducted on a 65x49x49 grid with algebraic stretching in the wall normal directions. The stretching was kept under 4% in all regions. Shown in fig.3(a-d) are the resolved scaled normalized variances in the velocities with corresponding values from a 33x65x65 LES using a Smagorinsky model (Madabhushi and Vanka [15]). The latter LES used very low resolution in the axial direction. A spectral method was used to compute the derivatives in this direction which could lead to significant aliasing errors. The net effect would be an overprediction of u'^2.

As can be seen, u'^2 compares favorably in the core region but the present simulation predicts a shifted peak with a lower value. The difference is also magnified by the fact the u'^2 could be highly overpredicted in the LES using algebraic model. Similar is the trend in case of v'^2 and w'^2. Shown in fig.3d is the variation of kinetic energy (resolved and subgrid combined) along with LES conducted by Madabhushia and Vanka [15]. As seen, there seems to be significant differences in the wall region. Further, unlike in the case of 10000 Reynolds number simulation, the subgrid kinetic energy does not even have a large peak in the near wall region.

Two point correlations along the axial direction was computed at three different locations. The first location is at the center line, the second location is at the midpoint of the center and one of the corners and the third location is the midpoint of the center and the wall along the wall bisector. The one dimensional velocity spectrum at these locations is plotted in Fig 4. The inertial spectrum that is expected is also shown. $G[K_x]$ is the Fourier transform of the filter function. The inertial range form of the energy spectrum would be the actual spectrum times the square of this function. The core region seems to have a range of wavenumbers in the Kolmogorov inertial range.

At a glance, it seems that the subgrid kinetic energy equation tries to account for unresolved turbulence in the near wall region better at a higher Reynolds number. This is puzzling, but could be explained on the grounds that the secondary flow patterns that are the prime cause of difficulty in modeling this flow have reduced amplitudes at higher Reynolds numbers. The instantaneous velocity vectors of the secondary flow pattern in the cross plane are shown in Fig 5.

The effects of secondary flow wane with increasing Reynolds number. It is further likely that the region of fully developed turbulence extends much closer to the wall in the higher Reynolds number case thus making the phenemenology of LES modeling more accurate.

In conclusion, it is seen that, at higher Reynolds number, the subgrid kinetic energy does have a tendency to capture significant amount of unresolved turbulence. While the quantitative agreement is fairly acceptable in the core region, this model also shows promise in the viscous sublayer and might need some near wall modifications for a better performance. At lower Reynolds numbers, the cross plane has secondary velocities which are recirculatory and cause significant problems. Further research into recirculatory flows at right angled corners using LES is required to modify the present model.

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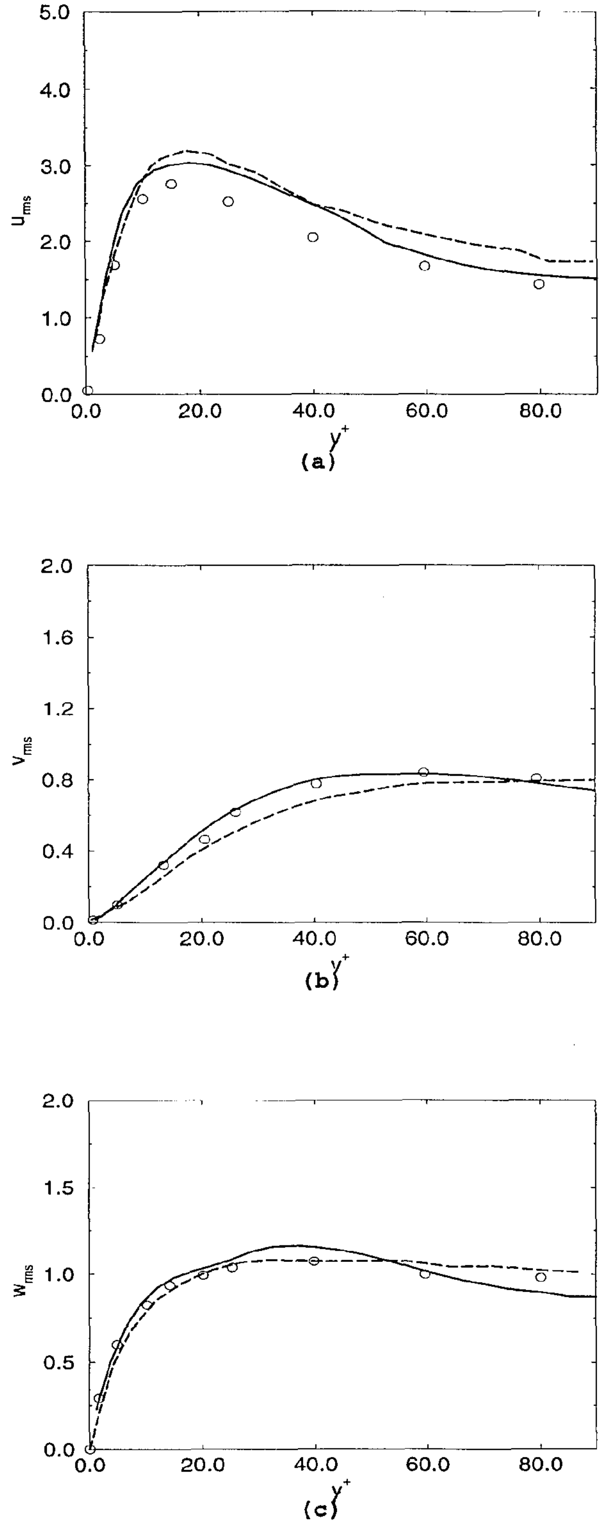

Figure 1: Comparison of rms velocity fluctuations at the mid–section of the duct.
Solid line:LES, dashed line:DNS(Huser and Biringen [11])
O: DNS (Kim and Moin [12])

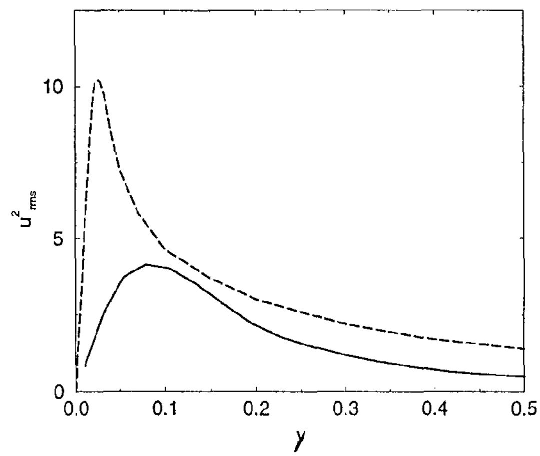

Figure.2a : Variation of axial velocity variance of along the wall bisector
——— LES, - - - - DNS (Huser et al.)

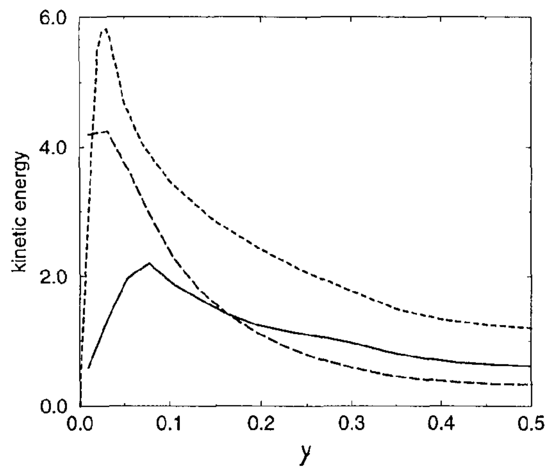

Figure.2b: Variation of turbulent kinetic energy along the wall bisector
——— LES(resolved),— — · LES(subgrid)
- - - - - DNS(Huser and Biringen [11])

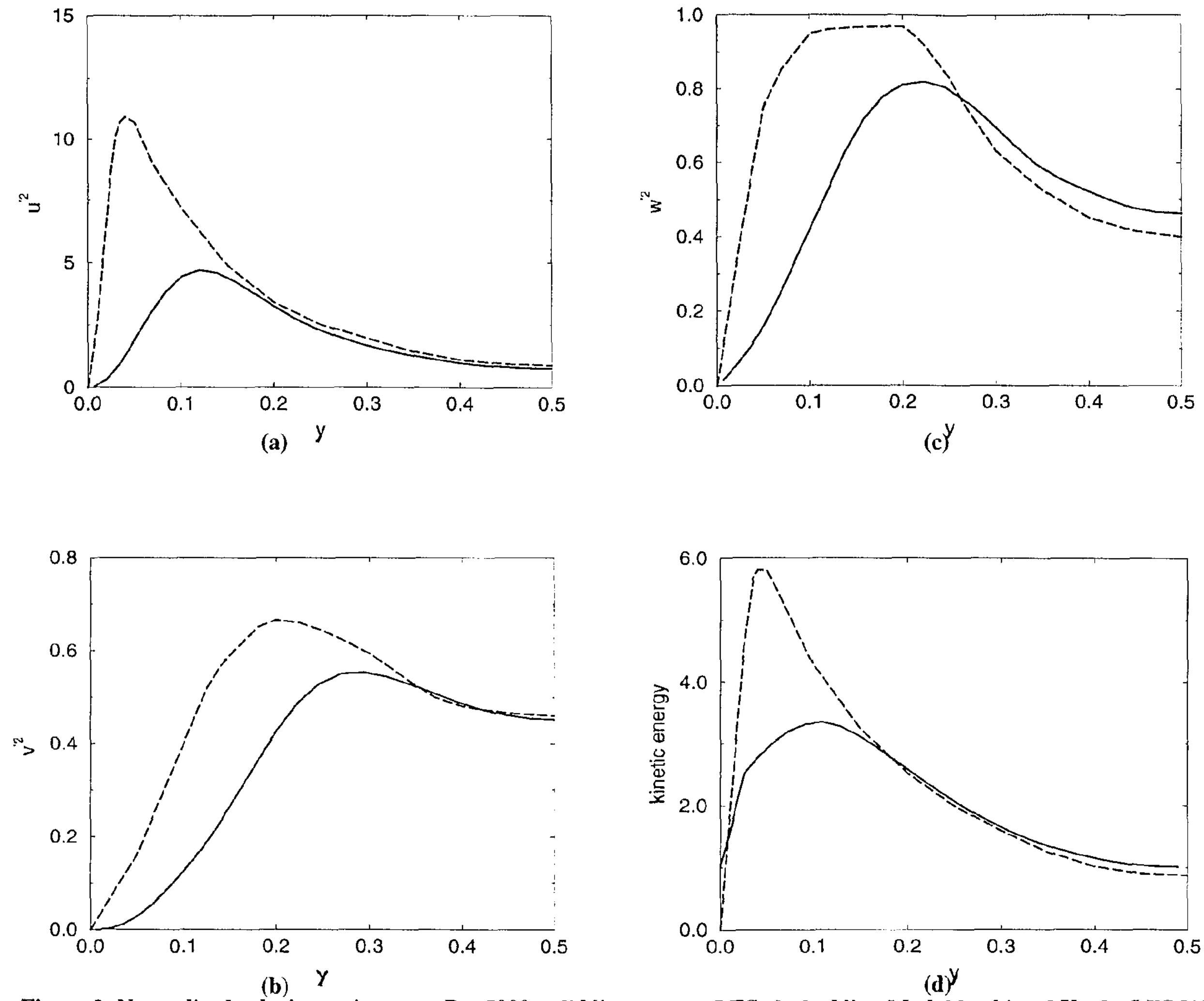

Figure 3: Normalized velocity variances at Re=5000, solid line:present LES, dashed line:Madabhushi and Vanka LES [15]

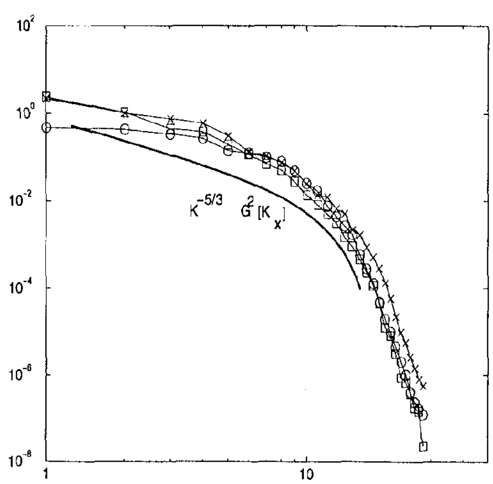

Figure 4: 1–D spectrum along the stream
❍ point 1, ❑ point2, x point 3

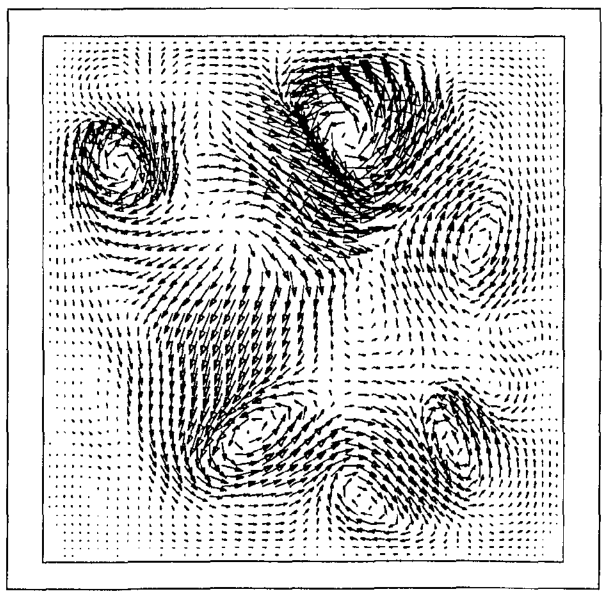

Figure 5: Instantaneous secondary velocity field in the cross–plane