Dynamics of Vortices in Numerically Simulated Turbulent Channel Flow

by

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ABSTRACT

The evolution of single hairpin vortices and multiple interacting hairpin vortices are studied in direct numerical simulations of channel flow at Re_τ=395. The purpose of this study is to observe the effects of increased Reynolds number and varying initial conditions on the growth of hairpins and the conditions under which single hairpins autogenerate hairpin packets. The hairpin vortices are believed to provide a unified picture of wall turbulence and play an important role in the production of Reynolds shear stress which is directly related to turbulent drag. The structures of the initial three-dimensional vortices are extracted from the two-point spatial correlation of the fully turbulent direct numerical simulation of the velocity field by linear stochastic estimation and embedded in a mean flow having the profile of the fully turbulent flow. The Reynolds number of the present simulation is more than twice that of the Re_τ=180 flow from earlier literature and the conditional events used to define the stochastically estimated single vortex initial conditions include a number of new types of events such as quasi-streamwise vorticity and Q4 events. The effects of parameters like strength, asymmetry and position are evaluated and compared with existing results in the literature. This study then attempts to answer questions concerning how vortex mergers produce larger scale structures, a process that may contribute to the growth of length scale with increasing distance from the wall in turbulent wall flows. Multiple vortex interactions are studied in detail.

DEDICATION

To my mother and father.

ACKNOWLEDGMENTS

It gives me great pleasure to remember and thank all the people who have guided me towards the successful completion of this scientific endeavor. Firstly, I would like to sincerely thank Prof. Ronald J. Adrian for his guidance and support during this work. Our discussions have inspired many a late night's worth of work. I also wish to thank Dr Marcus Hermann for his thoughts and ideas on this work. Valuable inputs from Dr B.J. Balakumar and Dr Kyoungyoun Kim are appreciated. The influence of Dr B.S.V Prasad Patnaik, Mr Ramachandran K.S, Mr Sundaram, Mrs Shobha Raman and Mr Kothandaraman M. is gratefully acknowledged with deep respect.

I would like to thank my parents Geetha and Parthasarathy and my brother Prashanth for their love, affection and wisdom. Talking to them seemed to solve many a problem. This work would not have been possible without them. I owe the deepest gratitude to my cousins Jana, Jayanthy and Karthik. The many conversations we have had were always a source of happiness and inspiration.

I had the pleasure of working with Jon Baltzer, Isaac Ziskin and Stefano Discetti during my stay at our laboratory. Their hardwork and knowledge served as a great source of motivation. I wish to thank Durella Donell for her timely help with the administrative work.

I also would like to thank Dr Gil Speyer, Dr Scott Menor and the entire high performance computing center for their assistance with running my simulations in the university's super computer.

Last but not the least, I wish to thank my friends who have always stood by me during the highs and lows I have had. They have been a great source of strength and encouragement throughout and our conversations had served as starting points of many a train of thought.

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LIST OF SYMBOLS

Symbol

A_{ik}	linear coefficients for stochastic estimation
h	half-channel height
i	unit imaginary number
j	component index
k	component index
k_x	streamwise wave number
k_y	wall-normal spectral mode number
k_z	spanwise wave number
l	component index
L_x	length of the computational box in the streamwise direction
L_z	length of the computational box in the streamwise direction
p	fluctuating pressure
rx	distance between x and x’
R_{jl}	two-point, second order spatial correlation tensor
Re_τ	Reynolds number based on wall friction velocity and half-channel height time
u	fluctuating velocity component in the streamwise direction
U	mean streamwise velocity
x	streamwise position
y	wall-normal position

z	spanwise position

Greek Symbols

γ_{II}	the angle between the event vector and the negative streamwise axis for quadrant II events
γ_{IV}	the angle between the event vector and the negative streamwise axis for quadrant IV events
υ	kinematic viscosity
ρ	density
τ_w	shear stress evaluated at the wall

Superscripts

+	denotes that the quantity is non-dimensionalized with viscous scales fluctuating quantity

Other Notation

<f>	denotes ensemble average of the quantity f

Chapter 1

INTRODUCTION

One of the most fundamental properties of wall turbulence is that the length scale, defined in various ways increases with distance from the wall. Starting with the mean spanwise spacing of low speed streaks at the wall, the length scale grows slightly through the buffer layer and then grows linearly throughout the logarithmic layer. This study attempts to answer the question on whether the vortex mergers would produce self similar vortices or a new class of structures. Channel flow was chosen since both experimental and theoretical investigations of complex turbulence interactions near the wall can be carried out.

Various studies by Bandhopadhyay (1980) and Smith (1984) ascertain the presence of vortex packets in the turbulent boundary layer. In this study, the vortex packet is shown to evolve out of single and multiple hairpin vortices generated through linear stochastic estimation. Hydrogen bubble and dye visualization by Haidari and Smith (1994) and inviscid models by Smith et al. (1991) attempted to address the natural formation of the vortex packets more closely. Although processes like vortex stretching and tilting were described by the inviscid models, a complete picture on vortex breakup and reconnection were not considered. Zhou, Adrian and Balachandar (1996) and Zhou, Adrian, Balachandar and Kendall (1999) performed direct numerical simulations in channel flow at Re_τ=180, and found that a single hairpin vortex is capable of creating successive upstream hairpins, providing that the strength of the first hairpin exceeds a critical value. This process, called 'autogeneration' leads to the

formation of a packet of hairpins travelling together, with the first hairpin being tallest and the last hairpin being shortest. The first hairpin generates a secondary hairpin, the secondary generates a tertiary, and so on for succeeding generations. If the initial hairpin is symmetric about a wall-normal plane through its middle, the resulting packet is also symmetric. But, if there is asymmetry, the hairpins assume the shape of a cane, and the packet structure tends to alternate from right-handed to left-handed canes. If the initial hairpin contains noise, the autogeneration leads to chaotic packets [Adrian (2007)]. Kim and Adrian (1999) proposed that the organization of hairpin vortices into packets and the interactions between these packets are characteristic features of wall turbulence that explain many observations like the large amount of streamwise kinetic energy residing in very long streamwise wavelengths. The formation of new streamwise vortices and the characteristic angles of inclined hairpins were further explained by Adrian, Meinhart and Tomkins (2000).

Hairpin vortex packets play an important role in the production of the Reynolds shear stress, which is directly related to the turbulent drag. Ganapathisubramani, Longmire and Marusic (2003) showed that about 25% of the total production of Reynolds shear stress in the log layer of turbulent boundary layers is attributed to vortex packets. In a hairpin packet, the total turbulent Reynolds stress can be thought of as arising from the incoherent component and the coherent component. The incoherent component is the sum of the momentum transfers by each individual vortex and the coherent component is the sum of the momentum transfers produced by vortex interactions. In addition

to the experimental observation of hairpin packets in instantaneous flow fields using particle image velocimetry (PIV), statistical evidence of hairpin packets has been reported by Christensen and Adrian (2001) and Hambleton, Hutchins and Marusic (2006). Zhou, Adrian and Balachandar (1996) used the direct Numerical simulation of the Navier-stokes equation to study the evolution of a hairpin vortex in a unidirectional mean flow obtained from the low-Reynolds number turbulent channel flow of Kim, Moin and Moser (1987). Their approach is adopted in the present study. The initial vortex structure without the presence of the other eddies (i.e. in a clean turbulent mean flow environment) has made it possible to visualize clearly the auto generation of new hairpin vortices.

1.1.Channel flow model

1.1.1 Geometry

The channel is composed of two infinite parallel walls, spaced a distance 2h apart. The streamwise and spanwise directions are $2\pi h$ and πh respectively (2480.6 and 1240.9 in wall units). The computation is carried out with 2113536 grid points (128 x 129 x 128, in x, y, z) for a Reynolds number of 395 based on the wall shear velocity u^*. The model assumes that the flow is periodic in the plane of the walls. Thus, a finite sized section can be used to model the infinite channel. The section used in this study is shown in Figure 1.1.

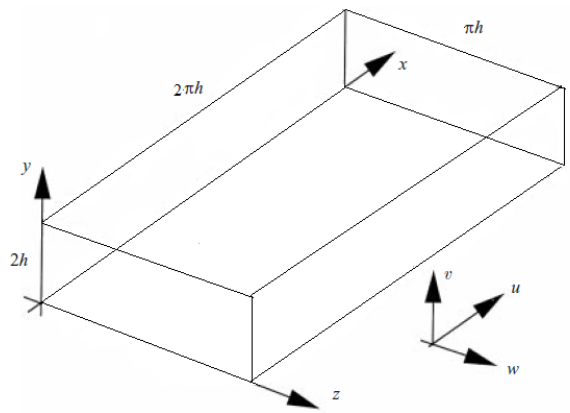


Figure 1.1 The channel geometry. The x, y and z coordinates show the streamwise, wall-normal and spanwise directions. The streamwise and spanwise directions are respectively 2πh and πh long which is 2480.6 and 1240.9 in wall units. The 2 infinite parallel walls are spaced 2h apart (790 wall units).

With this computational domain, the grid spacing's in the streamwise and spanwise directions are respectively $\Delta x^+ \approx 19.37$ and $\Delta z^+ \approx 9.69$ in wall units. Non-uniform meshes are used in the normal direction with $y_j = \cos\theta_j$, for $\theta_j = (j-1) \pi / (N - 1)$, $j = 1,2, ..., N$. Here N is the number of grid points in the y-direction.

1.1.2 Governing Equations

The initial turbulent flow field is evolved in time by solving the Navier Stokes equation along with the incompressibility condition. The equations used are the same as used in the thesis by Kendall (1992). Written in non-dimensional form, the equations can be represented as

$$\frac{\partial \tilde{u}^+}{\partial \tilde{x}} + \frac{\partial \tilde{v}^+}{\partial \tilde{y}} + \frac{\partial \tilde{w}^+}{\partial \tilde{z}} = 0 \qquad (1.1a)$$

$$\frac{\partial \tilde{u}^+}{\partial \tilde{t}} + \frac{\tilde{u}^+ \partial \tilde{u}^+}{\partial \tilde{x}} + \frac{\tilde{v}^+ \partial \tilde{u}^+}{\partial \tilde{y}} + \frac{\tilde{w}^+ \partial \tilde{u}^+}{\partial \tilde{z}} = -\frac{\partial \tilde{p}^+}{\partial \tilde{x}} + \frac{1}{\mathrm{Re}_\tau}\left\{\frac{\partial^2 \tilde{u}^+}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{u}^+}{\partial \tilde{y}^2} + \frac{\partial^2 \tilde{u}^+}{\partial \tilde{z}^2}\right\}$$

$$\frac{\partial v^+}{\partial \tilde{t}} + \frac{\tilde{u}^+ \partial v^+}{\partial \tilde{x}} + \frac{\tilde{v}^+ \partial v^+}{\partial \tilde{y}} + \frac{\tilde{w}^+ \partial v^+}{\partial \tilde{z}} = -\frac{\partial \tilde{p}^+}{\partial \tilde{y}} + \frac{1}{\mathrm{Re}_\tau}\left\{\frac{\partial^2 v^+}{\partial \tilde{x}^2} + \frac{\partial^2 v^+}{\partial \tilde{y}^2} + \frac{\partial^2 v^+}{\partial \tilde{z}^2}\right\}$$

$$\frac{\partial w^+}{\partial \tilde{t}} + \frac{\tilde{u}^+ \partial w^+}{\partial \tilde{x}} + \frac{\tilde{v}^+ \partial w^+}{\partial \tilde{y}} + \frac{\tilde{w}^+ \partial w^+}{\partial \tilde{z}} = -\frac{\partial \tilde{p}^+}{\partial \tilde{z}} + \frac{1}{\mathrm{Re}_\tau}\left\{\frac{\partial^2 w^+}{\partial \tilde{x}^2} + \frac{\partial^2 w^+}{\partial \tilde{y}^2} + \frac{\partial^2 w^+}{\partial \tilde{z}^2}\right\} \tag{1.1b}$$

$$\tilde{u}^+ = \frac{\tilde{u}}{u^*}$$

$$v^+ = \frac{v}{u^*}$$

$$w^+ = \frac{w}{u^*} \tag{1.1c}$$

In the governing equations, the channel half-height h is used as the length scale. Wall friction velocity $u^* = (\upsilon(\partial u/\partial y)_{y=\pm h})^{1/2}$ is used as the velocity scale. The characteristic pressure and time scales are ρu^{*2} and h/u^* respectively. This scaling results in the non-dimensional parameter of Reynolds number based on friction velocity, $Re_\tau = u^* h/\upsilon$.

1.2 Numerical Methods

1.2.1 Temporal and Spatial Discretization

Fourier expansions are used as part of the spectral collocation methodology for the periodic directions and a Chebyshev expansion is used for the non-periodic wall normal direction with Gauss-Lobatto points for spatial discretization. A time-splitting technique was employed for the decoupling of the pressure computations in the time advancement of the flow field. At each time

step, first an intermediate velocity field is computed with only the advection and diffusion effects taken into account. This intermediate velocity field is not divergence free. In the second step, an appropriate pressure is computed by solving a Poisson equation for pressure, based on which a pressure correction is applied to the intermediate velocity field to make it divergence free. Here, we employ a third order Runge Kutta scheme for the advection term and an implicit Crank Nicholson scheme for the diffusion term. The pressure effect is considered to be fully implicit in order to guarantee zero divergence at the end of the full timestep. The details of the numerical procedure used in this channel-flow simulation are elaborated in Kendall (1992).

1.2.2. Boundary conditions

The periodic conditions in the streamwise and spanwise directions are automatically satisfied by the use of fourier expansions. The no slip and the incompressibility conditions cannot be satisfied simultaneously because the time splitting scheme separates the momentum equation into two parts. In order to minimize the slip, a proper choice of the intermediate boundary condition must be made. The boundary condition for pressure is specified during the pressure-poisson step. It can be shown that a self-consistent, pure Neumann condition will allow slip velocity to be minimized.

1.2.3. Solution procedure

The Helmholtz equations for the three components of velocity are solved for each combination of horizontal Wave numbers to solve for the entire flow field. The equations are listed in Kendall's thesis (1992).

1.2.4. Grid Independence study

Grid refinement study was done for three different grids: 96x97x96, 128x129x128 (present grid) and 256x257x256. From figure 1.2, 128x129x128 grid is seen to be optimum for this computation since there is not much difference in λ_{ci} with the 256x257x256 grid. λ_{ci} , referred to as the swirling strength is the complex eigen value of the velocity gradient tensor ($D = \nabla u$) and it is a good measure of the vortex structure since it is frame independent and discriminates against shear layers which have vorticity but no swirling motion [Chong, Perry and Cantwell (1990), Chakraborty, Balachandar and Adrian (2006)]. t^+ is the non-dimensional time and is computed in equation 1.2. The change in time, dt is taken to be 1.25e-04 and the number of iterations is typically 10,000 although the value was increased for some computations to study the physics at a later time.

$$t^+ = \frac{dt \times \text{Number of iterations}}{(h/u^*)} \tag{1.2}$$

The swirling strength is obtained from the characteristic equation of the velocity gradient tensor which is given by

$$\lambda^3+P\lambda^2+Q\lambda+R=0 \tag{1.3}$$

Where, $P = -\text{div } u$; $Q= \frac{1}{2}[P^2-\text{tr}(DD)]$; and $R=-\det(D)$

Table 1.1 The threshold λ_{ci} for the 3 different grids at various t^+. λ_{ci} is the complex eigen value of the velocity gradient tensor and t^+ is the non-dimensional time computed from equation 1.2.

t^+	Maximum λ_{ci} (Grid: 96 x 97 x 96)	Maximum λ_{ci} (Grid: 128 x 129 x 128)	Maximum λ_{ci} (Grid: 256 x 257 x 256)
25	16.1136	60.6377	54.937
50	16.3566	65.3198	61.9359
100	18.5097	75.223	80.9264
150	21.9789	53.2664	55.0533
200	28.3971	54.1164	51.6953
250	26.3907	50.3841	50.4075
300	25.4552	51.8427	47.8462
350	25.7557	49.6056	48.9717
400	25.9998	43.6902	47.2204
450	25.747	39.759	44.3926
500	25.3215	33.3265	39.6914

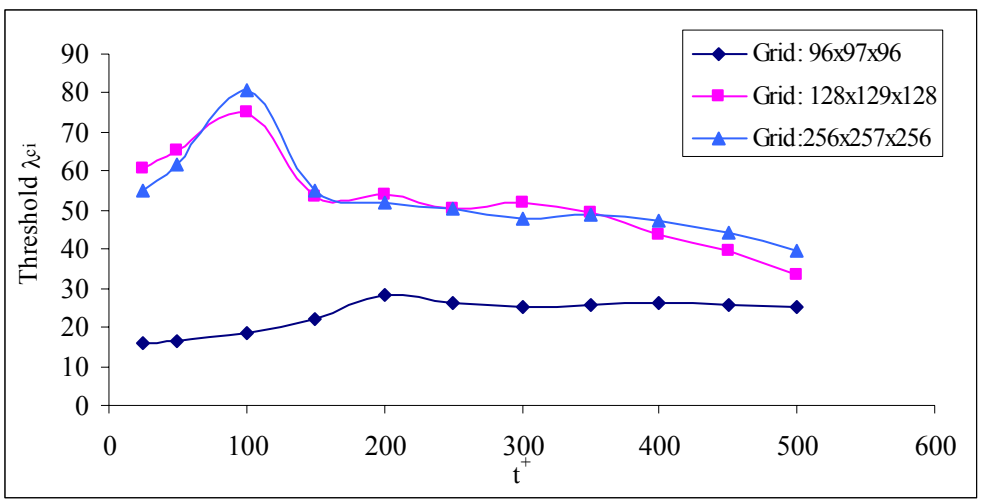
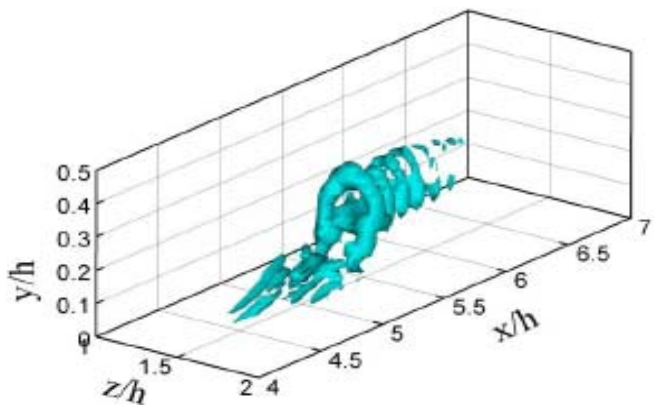


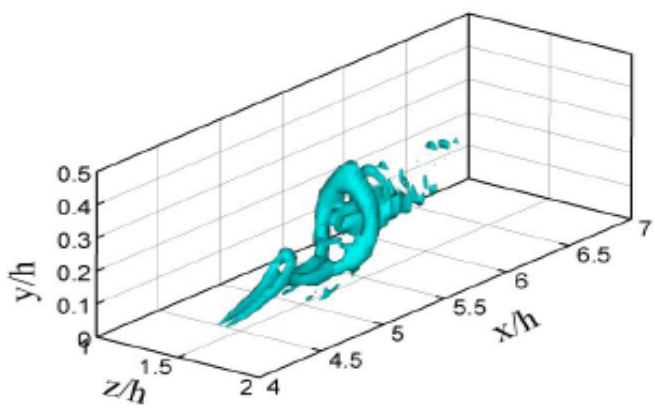
Figure 1.2 The plot between the threshold λ_{ci} and t^+ for the 3 different grids. λ_{ci} and t^+ are defined in equations 1.2 and 1.3 respectively and denote the complex eigen value of the velocity gradient tensor and the non-dimensional time.

The initial condition for figure 1.2 and 1.3 is defined as

$$u(x,t=0) = \langle u(x)|u'(y_m^+=46.6) = 3(u_m,v_m,0)\rangle \quad (1.4)$$



(a)



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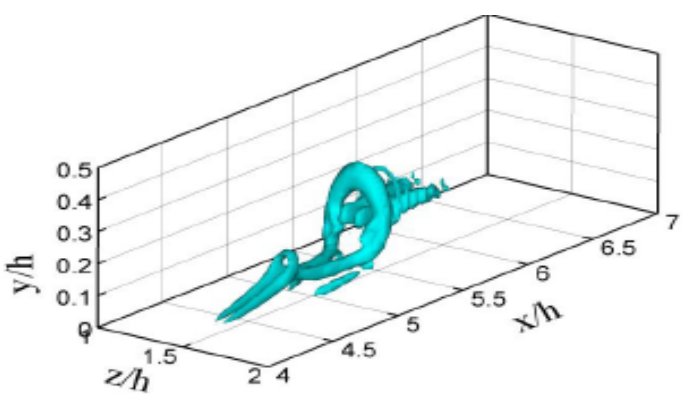


(c)

Figure 1.3 The evolved hairpin vortex structure at $t^+ = 250$ for (a) 96 x 97 x 96 grid; (b) 128 x 129 x 128 grid; and (c) 256 x 257 x 256 grid. (b) and (c) are qualitatively similar from the above figure. The initial condition is shown in equation 1.4.

The 1D streamwise correlations plotted as a function of the non-dimensionalized streamwise spacing (Δx^+) further shows the adequacy of grid (figure 1.5).

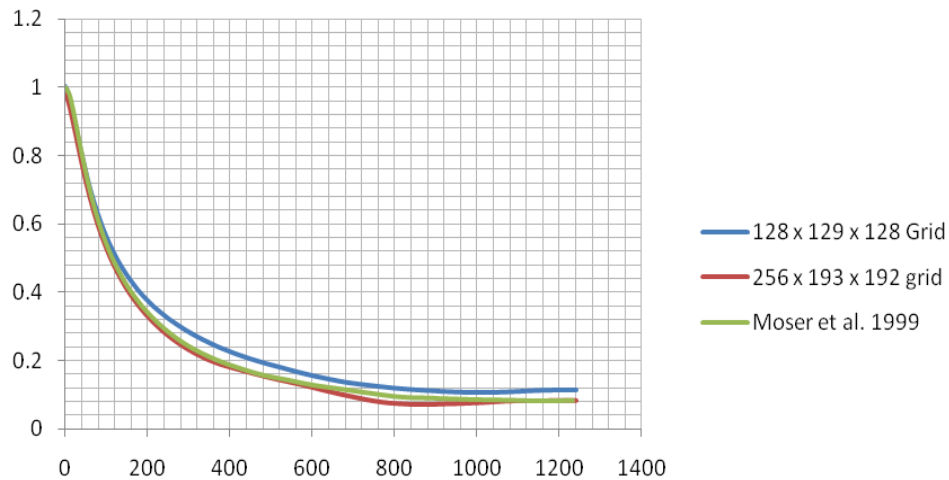


Figure 1.4 Plots of streamwise correlation vs the streamwise spacing. The correlation is defined in equation 1.5. R_{uu} is the streamwise correlation at (Δx^+, y^+=37.9,y'^+=37.9, Δz^+=0) and is non-dimensionalized with the correlation at zero streamwise spacing (Δx^+=0). These agree closely with the results of Moser, Kim and Mansour's (1999) computation on a finer grid (256x257x256).

A detailed discussion of the properties of the initial velocity fields and the initial structure extraction using linear stochastic estimation is given in chapter 2. In chapter 3, the evolution of a single hairpin vortex in the channel flow is discussed and the results are compared with literature. Multiple vortex interactions are studied in chapter 4. Finally, in chapter 5, the conclusions obtained from this research program are summarized and some recommendations for future work in the area of conditional vortex dynamics are given.

Chapter 2

METHODOLOGY

2.1 Turbulent mean properties

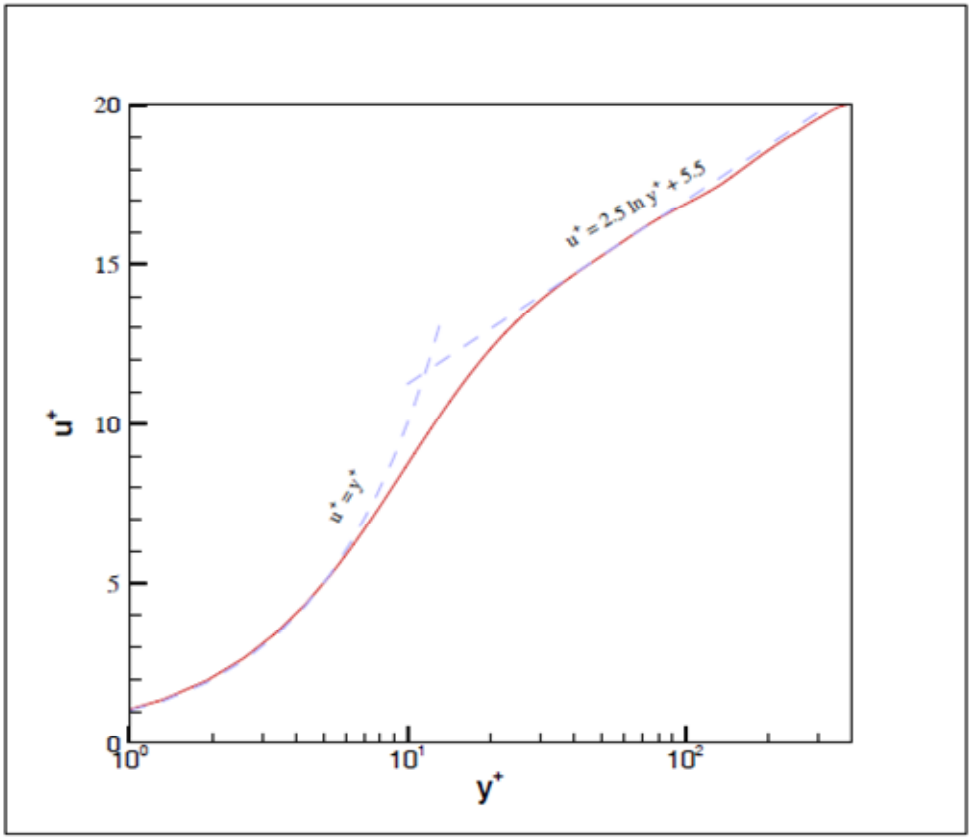


Figure 2.1 The mean velocity profile for the channel flow plotted with the law of the wall. The superscript + indicates a non-dimensional quantity scaled by the wall variables; $y^+ = yu^*/\nu$ is the viscous height of the channel where ν is the kinematic viscosity and $u^* = (\tau_w / \rho)^{1/2}$ is the wall shear velocity.

Starting from the initial velocity field, the governing equations were integrated forward in time until the numerical solutions reached statistically steady states. The calculations were considered to be complete when the time-averaged turbulence quantities became stationary. The profile of the mean velocity non-dimensionalized by the wall-shear velocity is shown in figure 2.1. The collapse of

the mean-velocity profiles corresponding to the upper and lower half of the channel indicates the adequacy of the sample taken here for the average.

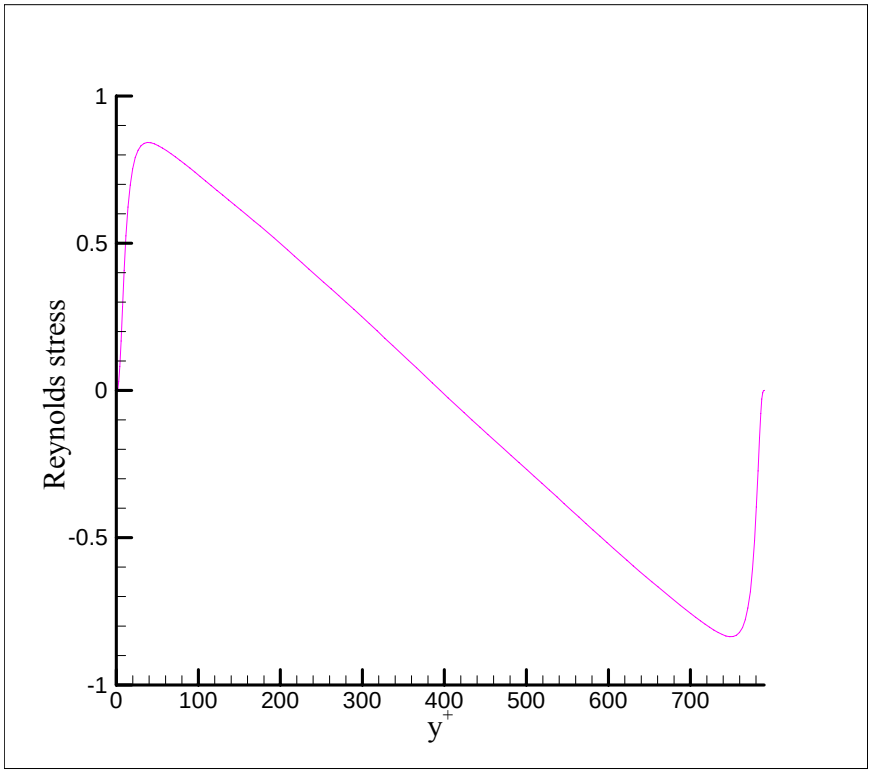


Figure 2.2 Vertical profiles of the resolvable mean Reynolds shear stress $\overline{uv}$. Re_τ=395. The grid adopted is 128 x 129 x 128. The stress was validated with the results of Moser, Kim and Mansour (1999) as shown in figure 2.4 a.

The profile in figure 2.2 indicate that the average Reynolds shear-stress profile has attained the equilibrium shape that balances the downstream mean pressure gradient in the regions away from the walls. In the vicinity of the walls, the viscous stresses are significant, and they, together with the total Reynolds stress, balance the mean pressure gradient. The symmetry of the profile about the channel centre line indicates that the total averaging time and statistical sample are adequate. The other characteristic properties of the flow, like the root mean square velocity were also plotted.

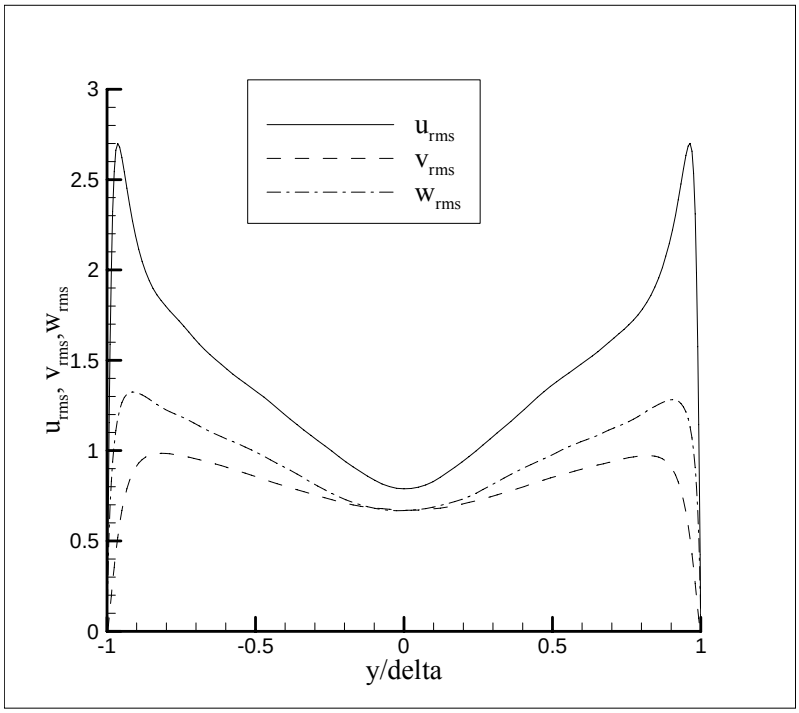
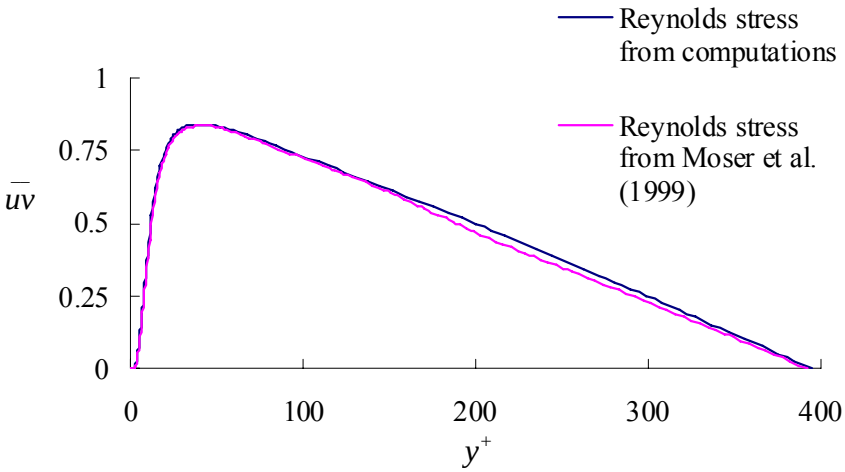
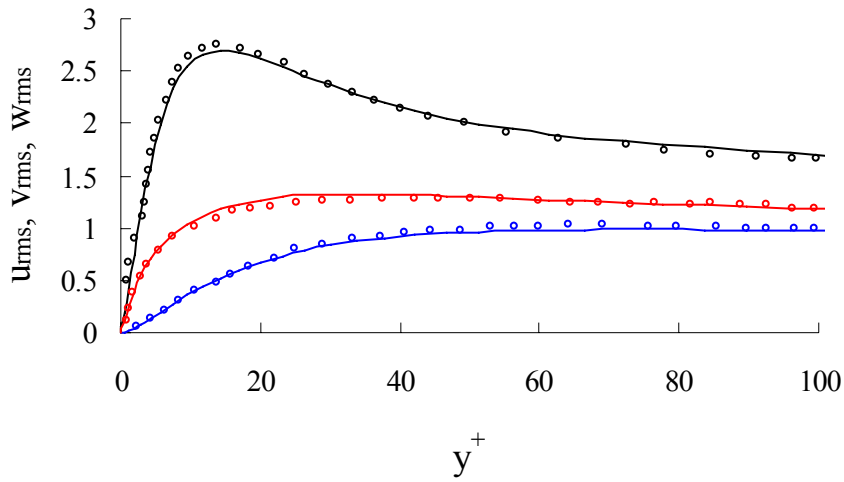


Figure 2.3 Plots of the root mean square components of velocity against the wall-normal distance normalized with Re_τ=395. Validation with the Re_τ=395 result of Moser, Kim and Mansour (1999) is shown in figure 2.4 b



(a)



(b)

Figure 2.4 Validation of computations with the Re_τ=395 results of Moser, Kim and Mansour (1999) (a) The magnitude of Reynolds stress obtained from the Reynolds stress tensor as a function of the non-dimensionalized wall-normal distance (y^+) upto y^+=395. (b) ___: u_{rms}, ___ : v_{rms}, ___ : w_{rms}. ° represents Moser et al.'s results for a finer (256 x 257 x 256) grid.

Once again, the symmetry of the calculated turbulence intensities about the centre line of the channel indicates that the total averaging time was sufficient for an adequate statistical sample. 2nd order statistics like skewness and flatness which are important parameters in a turbulent flow [Davidson (2007)] are defined as

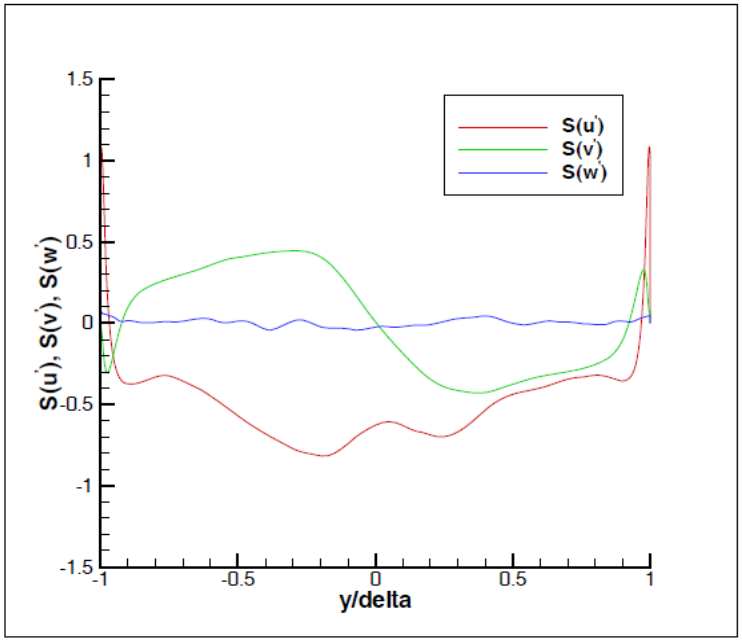
$$S = \frac{\overline{u_i^3}}{\overline{u_i^2}^{3/2}} \tag{2.1a}$$

(i=1,2,3; no summation)

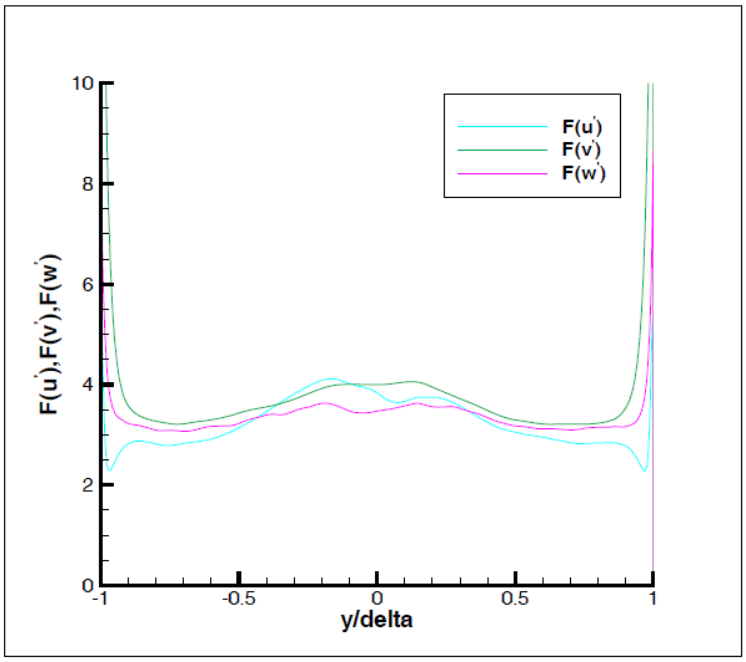
$$F = \frac{\overline{u_i^4}}{\overline{u_i^2}^{2}} \tag{2.1b}$$

The flatness factors of all the velocity components reach their maxima at the wall. This indicates that in the vicinity of the wall, the turbulence is highly intermittent. Throughout an appreciable portion of the channel cross-section, F(w') and S(w')

are approximately equal to three and zero respectively. These values correspond to the flatness and skewness factors of a Gaussian distribution. Near the wall, S(u') is positive, whereas away from the wall it is negative. This indicates that near the wall the large-amplitude u-fluctuations are primarily due to arrival of high-speed fluid from regions away from the wall. On the other hand, away from the wall the large-amplitude u-fluctuations are most probably associated with low-speed fluid leaving the wall region. This is encouraging considering the significant contribution of small-scale turbulence to these quantities and the difficulties associated with their measurements.



(a)



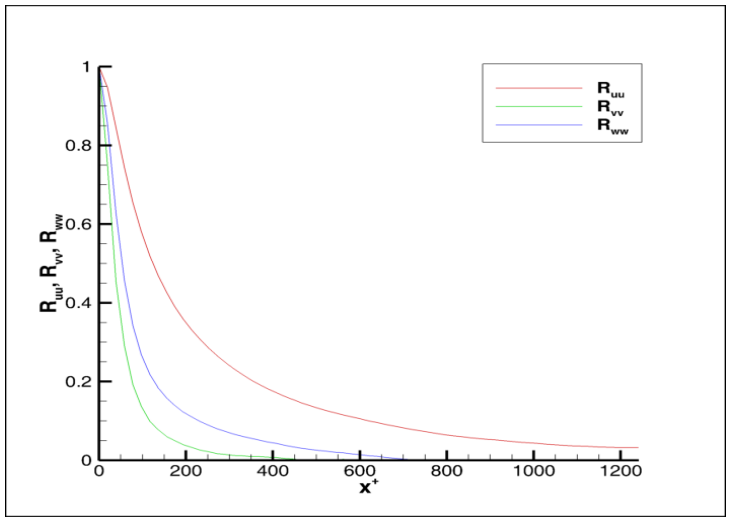
(b)

Figure 2.5 Plots of (a) Skewness and (b) Flatness for the channel flow data. u', v' and w' represent the velocity components in the streamwise, normal and spanwise directions respectively. S(w') and F(w') are predominantly 0 and 3 respectively.

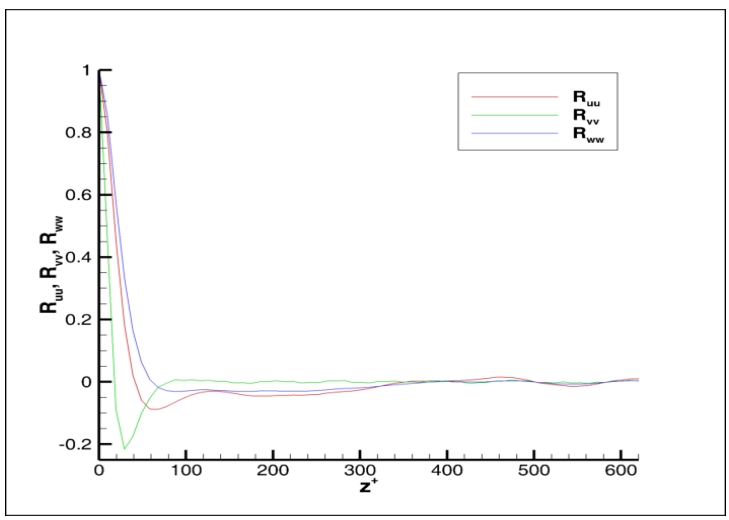
2.2 Correlation

In order to perform a linear estimate of the velocity field given a set of velocity conditions, the full two-point, second-order spatial correlation tensor, equation (2.2) is needed. This tensor was calculated using equation 2.2.

$$Rj_l(x,x') = \langle uj(x)\, u_l(x') \rangle \qquad (2.2)$$



(a)



(b)

Figure 2.6 Plots of velocity correlations as a function of the normalized (a) streamwise distance; (b) spanwise distance. R_{uu}, R_{vv} , R_{ww} are computed at (Δx^+, y^+=11.8, y'^+=11.8, Δz^+=0) and is non-dimensionalized by the correlation values at Δx^+=0.

These profiles show that, the longitudinal correlation in the streamwise direction extends over much longer distances than do all other correlations. The slow decay of R_{uu} with increasing x^+ indicates that near the wall, the eddies are highly

elongated in the streamwise direction. On the other hand, the profiles of figure 2.4 (b) shows that the spanwise extent of turbulence structures near the wall is much smaller than for those away from the wall. It hence appears that, near the walls the computed flow field consists of elongated streaky structures.

2.3 Joint Probability Distribution functions

The streamwise and wall normal velocity components of the event vector are chosen based on their contribution to mean Reynolds shear stress. The events, u(x,t=0), studied in this work are chosen such that the product of the simultaneous Reynolds stress and the probability of occurrence of events are maximized[(Moin, Adrian and Kim (1987)] Second (Q2) and fourth quadrant (Q4) events are studied.

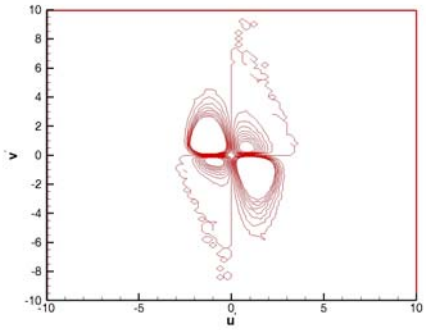
Table 2.1 Quadrant IV events which maximize the product of Reynolds stress and Probability of occurrence [Moin, Adrian and Kim (1987)]. u_m and v_m denote the maximum values of fluctuating u and v velocities; σ_u and σ_v denote the variances in the u and v direction.

Q4 event				
u_m/σ_u	v_m/σ_v	$u_m v_m/\sigma_u\sigma_v$	$\mathrm{Tan}^{-1}(u_m v_m/\sigma_u\sigma_v)$ degrees	y^+
1.2	-0.8	-0.58	-33.67	11.8
1	-1	-0.78	-44.98	46.6
1.2	-1	-0.69	-39.78	66.6
1.2	-1.2	-0.78	-44.98	109
1	-1	-0.78	-44.98	217
0.8	-0.8	-0.78	-44.98	395

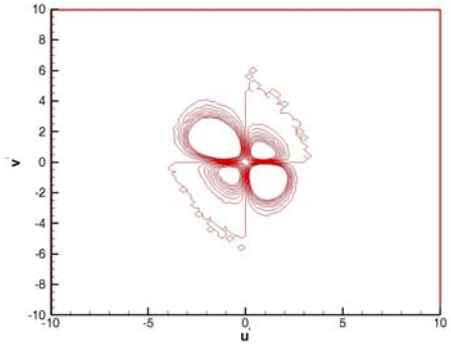
Table 2.2 Quadrant II events which maximize the product of Reynolds stress and Probability of occurrence [Moin, Adrian and Kim (1987)]

Q2 event				
u_m/σ_u	v_m/σ_v	$u_m v_m/\sigma_u\sigma_v$	$\mathrm{Tan}^{-1}(u_m v_m/\sigma_u\sigma_v)$ degrees	y^+
-1.4	0.8	-0.51	-80.25	11.8
-1.6	1.4	-0.71	-91.63	46.6
-1.4	1.4	-0.78	-80.18	66.6
-1.4	1.2	-0.70	-80.18	109
-1.4	1.4	-0.78	-80.18	217
-1	1	-0.78	-57.27	395

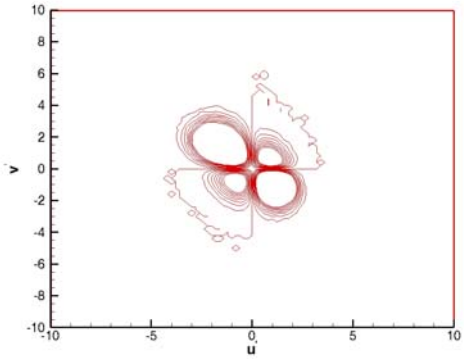
All the following plots are contour plots of <u'v'>*probability density function at various values of y^+.



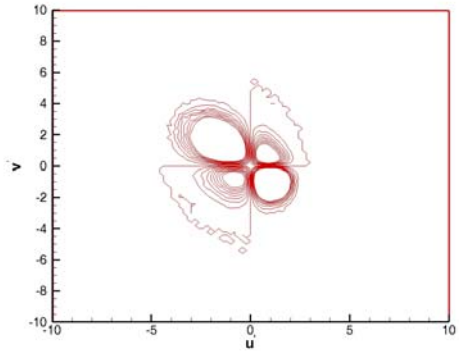
(a)



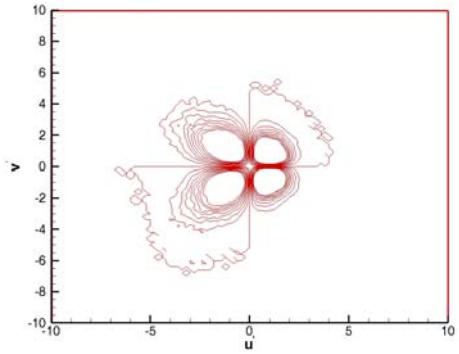
(b)



(c)

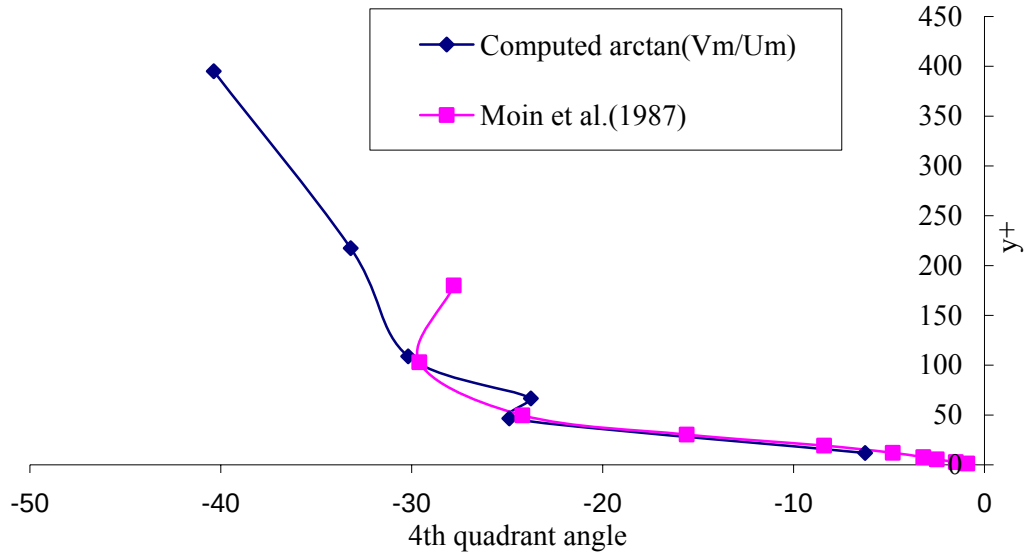


(d)

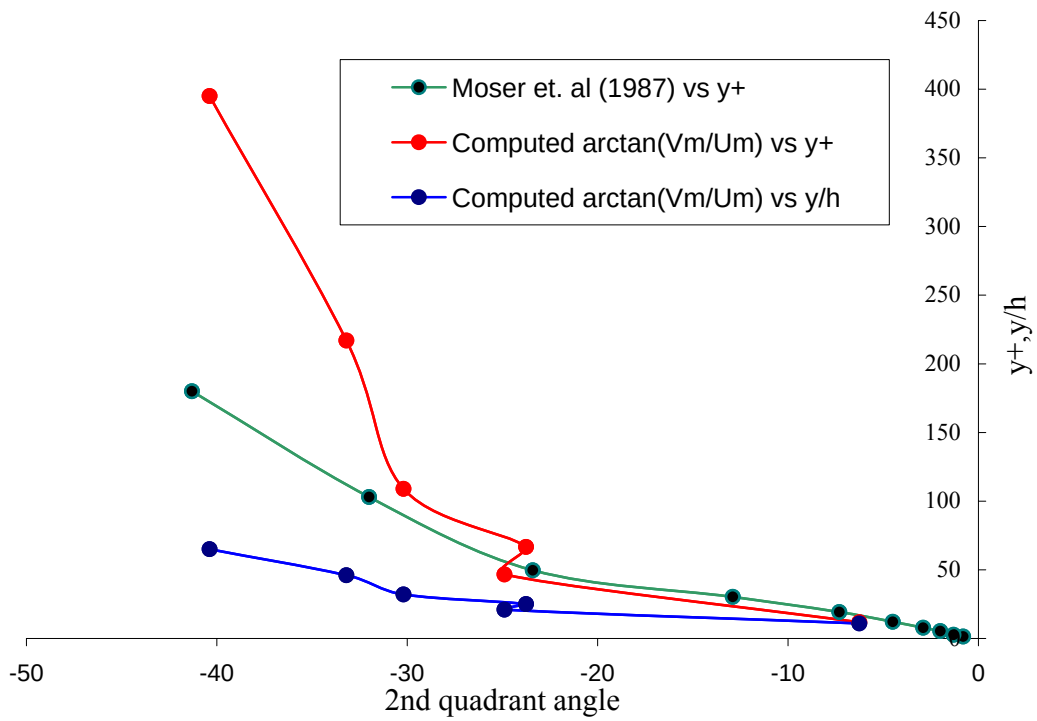


(e)

Figure 2.7 Joint probability distributions at various y^+ values (a) y^+=11.8; (b) y^+ = 46.6; (c) y^+= 66.6; (d) y^+= 109; (e) y^+ = 217; (f) y^+ = 395



(a)



(b)

Figure 2.8 Plots of (a) y^+ vs 4th quadrant angles (in degrees) and (b) y^+ and y/h vs 2nd quadrant angles (in degrees).The plots are validated with the results of Moin, Adrian and Kim (1987). The 4th and 2nd quadrant angles were obtained from table 2.1 and 2.2 respectively. These angles make the maximum contribution to the Reynolds stress tensor. The present computations were done at Re_τ=395 and Moin et al's results were at Re_τ=180

As is seen from figure 2.8, the profiles for Re_τ=395 agree well with Re_τ=180 [Moin, Adrian and Kim (1987). But there is deviation away from the wall. (y^+>100). The abrupt change in the flow angle which occurs in the buffer layer indicates transition from streamwise oriented wall layer structures to hairpin vortices characterizing the outer layer.

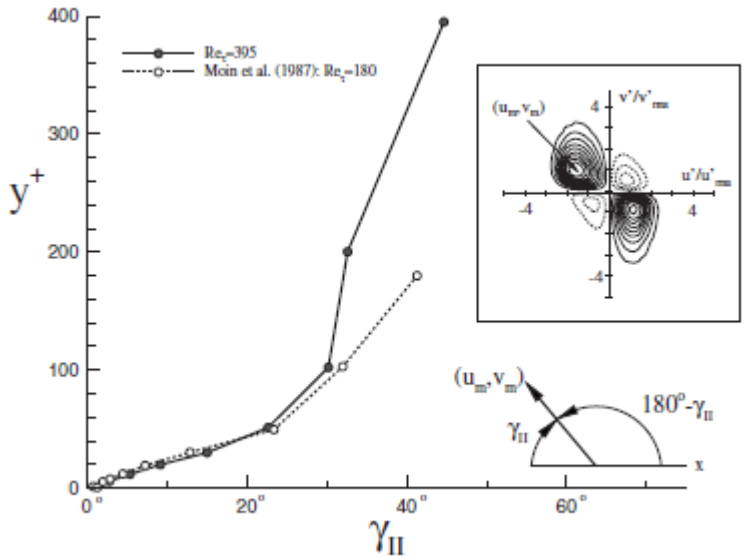


Figure 2.9 The angle of the Q2 vector as a function of distance from the wall obtained from Kim, Moin and Moser (1987). Inset: Method of defining the Q2 event (u_m,v_m,0)

2.4 Linear Stochastic estimation

Stochastic estimation is a simple procedure by which conditional averages are approximated in terms of unconditional correlation functions (Moin, Adrian and Kim). Linear stochastic estimation is accomplished by expressing the conditional average as a linear function of its data and solving a set of linear algebraic equations for the expansion coefficients. The initial condition consists of a

conditional vortex or a set of conditional vortices superposed onto a turbulent mean velocity profile. The conditional vortex is evaluated using Linear Stochastic estimation. The estimation procedure is briefed in Zhou, Adrian, Balachandar and Kendall (1999) and is described in detail in the appendix at the end of the current study. The choice of a symmetric Q2 event vector results in a vortical structure that resembles a near-wall quasi-streamwise vortex pair when the event is specified close to the wall and resembles a hairpin vortex when the event is specified sufficiently far away from the wall [Moin, Adrian and Kim (1987)]. The linear estimate of the conditional average $\langle u(x',t)|u(x,t)\rangle$ is calculated from equation (2.3) where A_{jk} are the estimation coefficients. For each value of the component j, the A_{jk} are determined by solving the 3x3 linear algebraic equations shown in equation (2.4). The location in the homogenous directions, x and z, may be selected arbitrarily and each estimate is evaluated for a given value of y as a function of the distance r=x'-x.

$$u_j(x',t) = A_{jk}(x',x)\, u_k(x,t) \tag{2.3}$$

$$R_{kl}(x,x')\, A_{jk}(x,x') = R_{lj}(x,x') = R_{lj}(r,y) \qquad j,k,l = 1,2,3 \tag{2.4}$$

By virtue of being extracted from the correlation tensor, the initial structure has length scales, shape and vorticity consistent with eddies that occur in the fully turbulent channel flow.

2.5 Vortex visualization

According to Zhou, Adrian and Balachandar (1996), a vortex usually refers to a tube-like structure with persistent and coherent rotation about its spine. Robinson

(1991) definition of a vortex explains the inadequacy of mathematical quantities like helicity and vorticity to characterize a vortex. On the other hand, a number of techniques for the identification of vortices have been proposed. Although a variety of techniques have been used in the past, the method of Chong, Perry and Cantwell (1990) is used in the current study due to the advantages which include frame independence and the display of shear layers which have vorticity but no swirling motion. The choice of λ_{ci} for this study was made so that the various vortical structures would be easily identifiable with minimal background noise, eliminating sensitivity dependence.

Table 2.3 Initial conditions used in this study for single vortex evolution. All computations were done at Re_τ=395 for 128 x 129 x 128 grid.

Run	X=(x+,y+,z+)	u=(u,v,w)	Movie location folder (on DVD)	Figure number
1	(0,46.6,0)	(-1.6,1.4,0)	Strength=1	1a
2	(0,46.6,0)	(-2,1.75,0)	Strength=1.25	1b
3	(0,46.6,0)	(-2.4,2.1,0)	Strength=1.5	1c
4	(0,46.6,0)	(-3.2,2.8,0)	Strength=2	1d
5	(0,46.6,0)	(-4,3.5,0)	Strength=2.5	1e
6	(0,46.6,0)	(-4.8,4.2,0)	Strength=3	1f
7	(0,46.6,0)	(-6.4,5.6,0)	Strength=4	1g
8	(0,11.8,0)	(-4,3.5,0)	y+=11.8	2a
9	(0,66.6,0)	(-4,3.5,0)	y+=66.6	2b
10	(0,217,0)	(-4,3.5,0)	y+=217	2c
11	(0,395,0)	(-4,3.5,0)	y+=395	2d
12	(0,46.6,0)	(4,-3.5,0)	Q4	3a
13	(0,46.6,0)	(-4,3.5,0)	Beta=0.2	4a
14	(0,46.6,0)	(-4,3.5,0)	Beta=0.4	4b
15	(0,46.6,0)	(-4,3.5,0)	Beta=0.5	4c
16	(0,46.6,0)	(-4,3.5,0)	Beta=0.6	4d
17	(0,46.6,0)	(-4,3.5,0)	Beta=0.8	4e
18	(0,46.6,0)	(-4,0,0)	u00	5a
19	(0,46.6,0)	(0,3.5,0)	0v0	5b

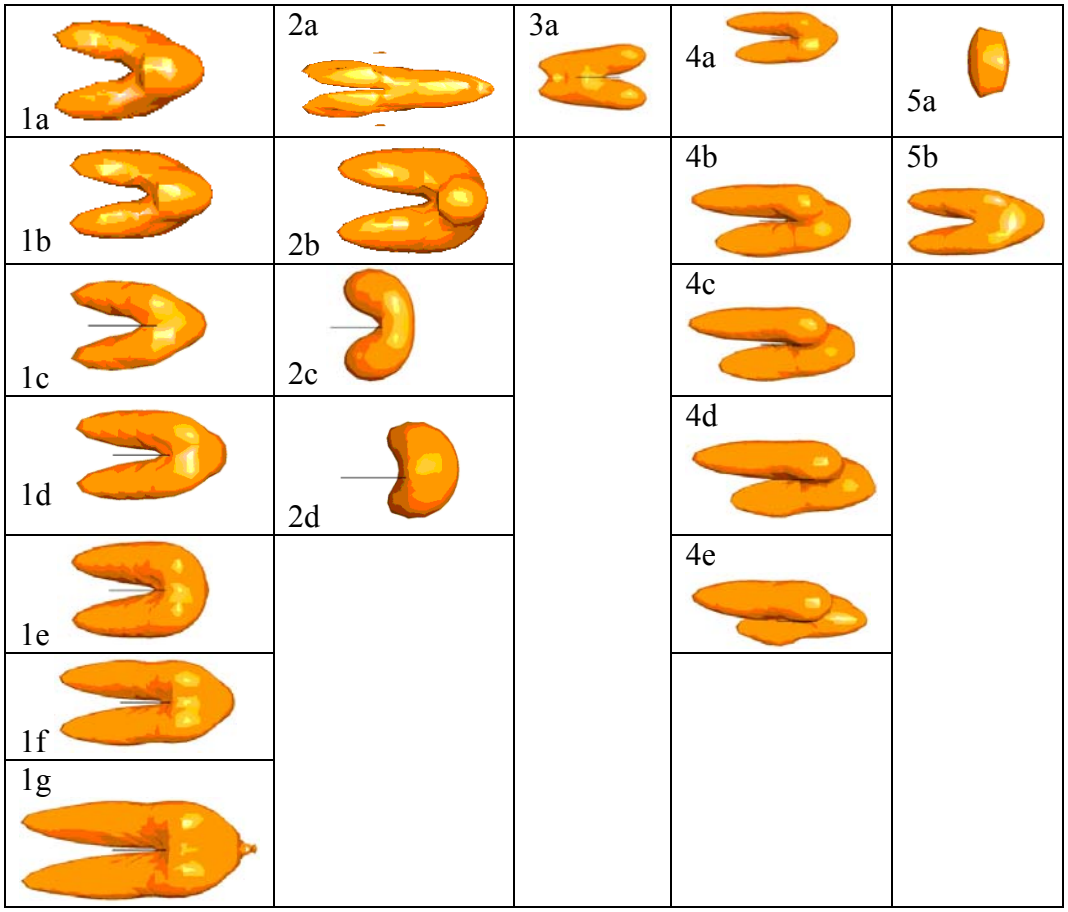


Figure 2.10 List of figures showing initial vortex shapes. Mathematical representation shown in table 2.3.

Table 2.4 Initial conditions used in this study for vortex interactions. All computations were done at Re_τ=395 for 128 x 129 x 128 grid.

Run	X=(x,y,z)	u=(u,v,w)	Movie location (on DVD)	Figure number
1	(0,46.6,0) (100,46.6,0)	(-4,3.5,0) (-4,3.5,0)	Streamwise vortex interaction	7a
2	(0,46.6,0) (100,46.6,0)	(-4,3.5,0) (-3.2,2.8,0)	Decreasing strength	7b
3	(0,46.6,0) (100,46.6,0)	(-4,3.5,0) (-4,3.5,0)	Increasing strength	7c
4	(0,46.6,0) (0,46.6,100)	(-4,3.5,0) (-4,3.5,0)	Spanwise vortex interaction	8a
5	(0,46.6,0) (100,46.6,0) (200,46.6,0)	(-4,3.5,0) (-4,3.5,0) (-4,3.5,0)	3 vortices/same strength	9a
6	(0,46.6,0) (100,46.6,0) (200,46.6,0)	(-4.8,4.2,0) (-4,3.5,0) (-3.2,2.8,0)	3 vortices/decreasing strength	9b
7	(0,46.6,0) (100,46.6,0) (200,46.6,0)	(-3.2,2.8,0) (-4,3.5,0) (-4.8,4.2,0)	3 vortices/increasing strength	9c
8	(0,46.6,0) (100,46.6,0)	(-4,3.5,0) (-4,3.5,0)	21_11	10a
9	(0,46.6,0) (100,46.6,0)	(-4,3.5,0) (4,-3.5,0)	1Q2Q4	11a
10	(0,46.6,0) (100,46.6,0)	(4,3.5,0) (4,-3.5,0)	1Q4Q2	11b
11	(0,46.6,0) (0,46.6,100) (0,46.6,200) (100,46.6,50) (100,46.6,150)	(-4,3.5,0) (-4,3.5,0) (-4,3.5,0) (-4,3.5,0) (-4,3.5,0)	Staggered	12a

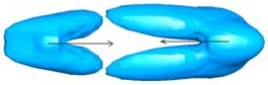
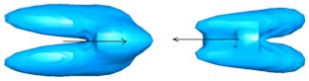
 7 a	 7 b	 7 c
 8 a		
 9 a	 9 b	 9 c
 10 a		
 11 a	 11 b	
 12 a		

Figure 2.11 List of figures showing initial vortex shapes. Mathematical representation shown in table 2.4.

Chapter 3

SINGLE VORTEX EVOLUTION

Zhou, Adrian, Balachandar and Kendall (1999) studied the evolution of a symmetric pair of quasistreamwise vortical structures extracted from the two-point correlation tensor of turbulent channel flow data by linear stochastic estimation procedure. The initial structure evolves into a hairpin-like vortical structure which can, in turn, generate streamwise vortices, thus providing a mechanism for continual regeneration of new vortices.It is recognized that the strength of the initial structure can play an important role, especially in the nonlinear stages of the evolution. Therefore, the effect of strength on vortex evolution is considered in section 3.1. Also, in the present study, the wall normal location, y^+ of the event vector will be varied from near the boundary to the middle of the channel (section 3.2).The symmetric event vector is specified as $u = \alpha u_m$, $v = \alpha v_m$ and $w = 0$, where the multiplicative factor α referred as 'strength' of the initial structure, is varied from 1.0 to 3.5. Zhou et al.(1999) showed that asymmetric initial vortices grow more rapidly than symmetric ones and hence are likely to be the most common form found in natural wall turbulence. The effect of asymmetry for various values of β is shown in section 3.3. Section 3.4 discusses the evolution of a single vortex into a fully turbulent field.

3.1 Effect of strength

Kim, Sung and Adrian (2008) examined the autogeneration process by which new hairpin vortices are created from a sufficiently strong hairpin vortex, leading to the formation of a hairpin packet. It is observed that while stronger initial vortices result in the formation of a hairpin packet, weaker initial vortical structures, which live long and maintain their integrity, do not participate in the autogeneration of additional hairpins. Owing to the linear nature of the estimation procedure, the entire velocity field of the initial structure scales linearly with α. As the strength of the initial event vector α is changed, the initial structure always rolls-up into a hairpin vortex, but its strength and accordingly its subsequent evolution differs. The main effect is on the length of the resulting hairpin vortex along the streamwise direction. The formation process of the primary hairpin vortex remains the same qualitatively. Whereas the initial structure evolves into an Ω-shaped primary vortex, irrespective of its initial strength α, and initial location y^+, the autogeneration of secondary and tertiary vortices is quite sensitive to the amplitude. From the following figure, it appears that the threshold amplitude reaches a minimum for an initial location y^+ of around 30.

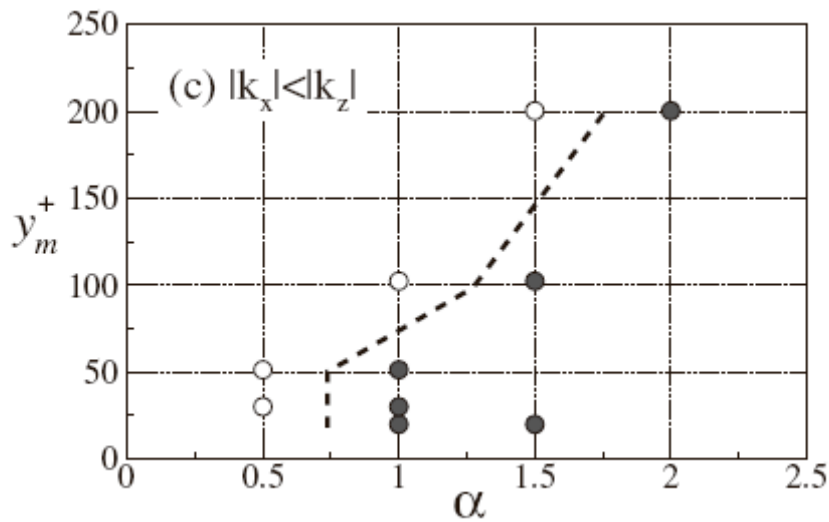
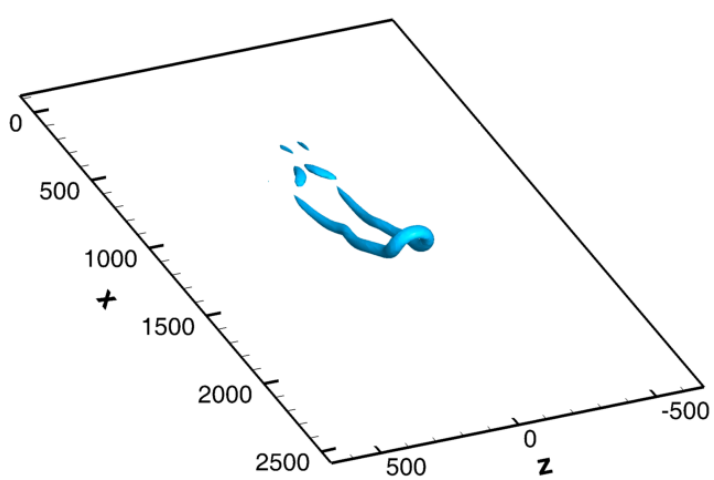


Figure 3.1 Generation of secondary hairpin vortices depends on the strength of initial vortical structures and location of the event vector used to extract the initial vortical structure. (•) Case with new hairpins. (°) Case without new hairpins [Kim, Sung and Adrian (2008)].

Computations were done to see if the downstream vortex affects the upstream vortex in autogeneration. From figure 3.1, the threshold for auto-generation for Re_τ=180 is between 0.5 and 1, though there is no auto-generation evident at α=1 for Re_τ=395. Auto-generation for Re_τ=395 exists between α=1.25 and α=1.5. Figure 3.2 shows the hairpin structure at t^+=150 for various strengths.



(a)

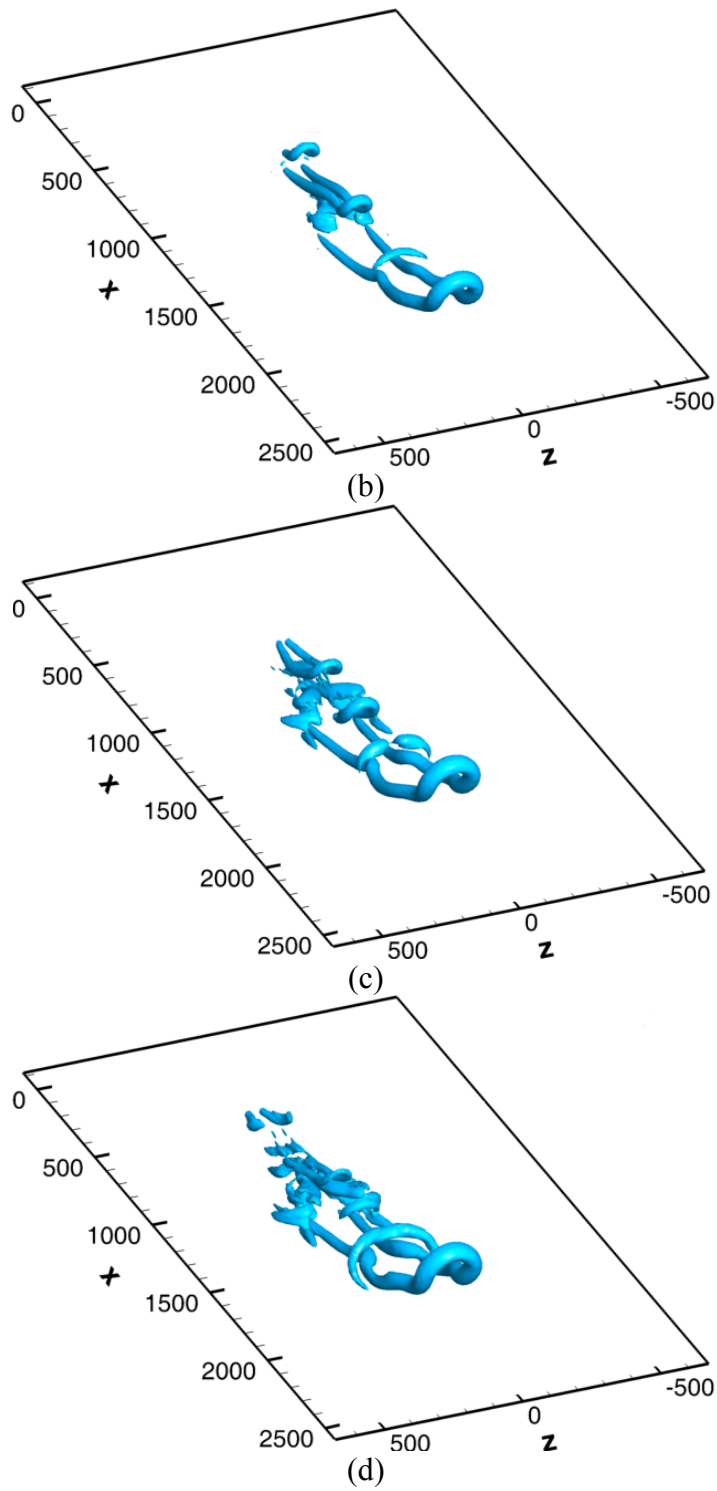


Figure 3.2 Vortex evolution at t^+=150 for different strengths (a)α=2; (b) α=2.5; (c) α=3; (d) α=3.5. The initial velocity field specified was $u=\alpha(u_m,v_m,0)$ where u_m and v_m were obtained from the joint probability density function and were taken to be (-1.6,1.4,0)

Even though the growth of the vortices tends to be qualitatively similar for all strengths greater than the threshold strength, the disturbances (or the tongue) in the downstream side of the primary vortex are more pronounced as we increase the strength. These disturbances can be considered as numerical errors and are hence more visible as we increase the values of fluctuating u and v velocities.

Table 3.1 The time (t^+) taken for the vortex to disappear when a sub-critical strength is used for computation. These computations were done at y^+=46.6. x^+ denotes the non-dimensionalized streamwise spacing.

t^+	x^+ (strength = 1)	x^+ (strength = 1.25)	x^+ (strength = 1.5)	x^+ (strength = 3)
25	200	200	200	360
50	240	280	320	560
150		240	400	1280
175		120	360	2380
200		80	280	
500			440	
650			680	
800			280	
900				

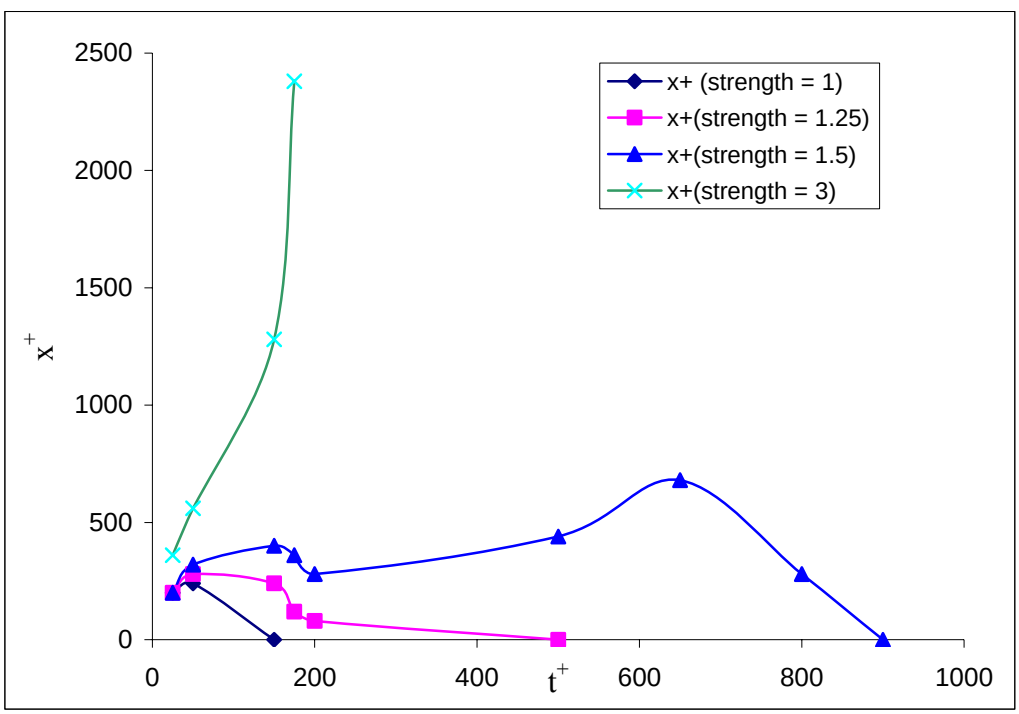


Figure 3.3 A comparison between the lengths of the eddy (x^+) at various t^+ values.

The hairpin vortex at alpha =1 disappears very quickly as can be seen from figure 3.3. Increasing the strength makes the length of the hairpin grow faster.

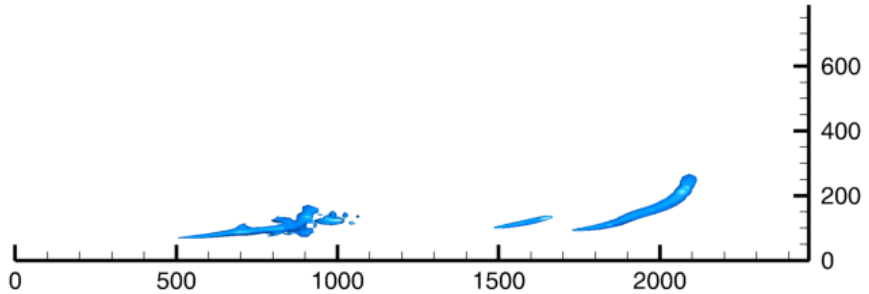
3.2 Effect of y-normal position

The choice of a symmetric Q2 event vector results in a vortical structure that resembles a near-wall quasi-streamwise vortex pair when the event is specified close to the wall and resembles a hairpin vortex when the event is specified sufficiently far away from the wall [Moin, Adrian and Kim (1987)].

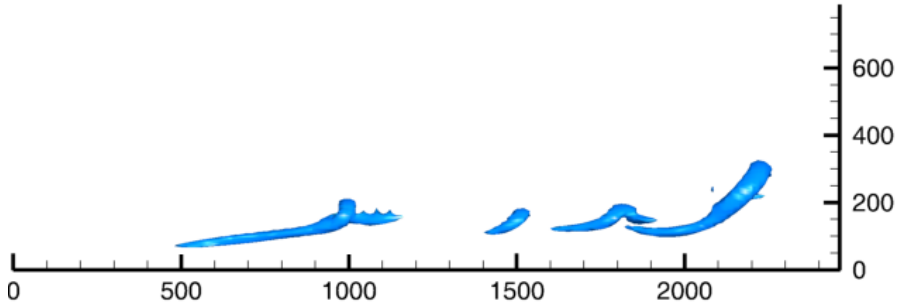
It can be observed that there exists a bridge of vorticity across the two streamwise vortices at the point where the event vector is specified. The strength of the bridge is weak when the event vector is close to the wall but is relatively stronger when the event vector is farther away from the wall. The average inclination of the initial structure decreases (or increases) as the *y*-location of the event vector is lowered (or raised), but the spanwise separation at the upstream end remains at about 100 viscous wall units approximately independent of y^+ . This is consistent with the accepted mean low-speed streak spacing of about 100 viscous wall units in the near-wall region. The location of the spanwise bridge is slightly upstream of the downstream tip of the quasi-streamwise vortices. In other words, the quasi-streamwise vortices extend slightly beyond their spanwise bridge. The spanwise bridge becomes stronger as the location of the event vector, y^+ increases and the initial structure resembles more closely a hairpin vortex.

The presence of an optimum distance from the wall for the initial structure can be explained as followed. The optimum distance is a balance between self- and

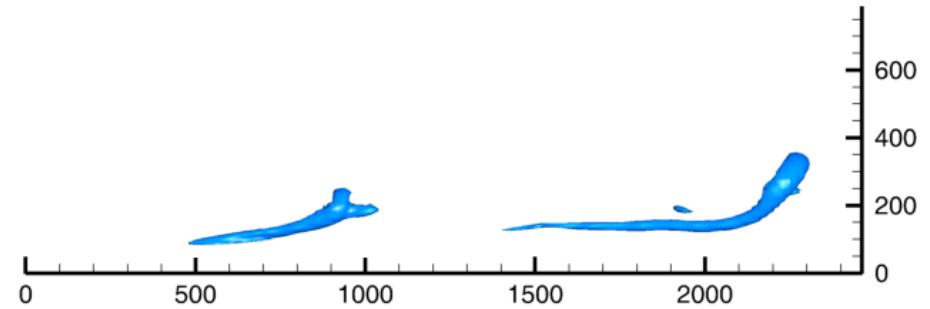
mutual-induced motion of the quasi-streamwise vortex legs which tends to lift-up and curl back the vortices and the influence of mean shear which stretches along the streamwise direction and intensifies the vortices. Very close to the wall, viscous effects are also important. The enhanced viscous effects result in an increase in the threshold amplitude for initial vortices starting very close to the boundary. Away from the wall, the induced motion is determined by the strength of the vortex structure and streamwise stretching by the mean shear. With increasing distance from the wall, the mean shear rapidly reduces, thereby decreasing the intensification of the initial vortex structure by stretching. Thus, an initial hairpin vortex farther away from the boundary needs to be of sufficiently higher strength to generate subsequent hairpin vortices.



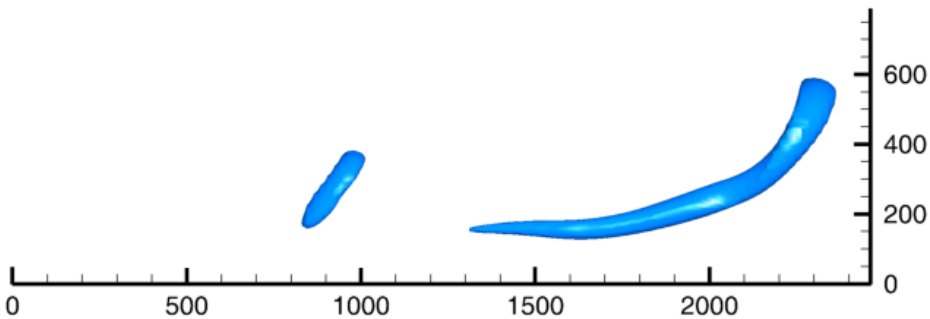
(a)



(b)



(c)



(d)

Figure 3.4 Evolution of the hairpin vortex at various values of y^+; (a) $y^+ = 11.8$; (b) $y^+ = 46.6$; (c) $y^+ = 66.6$; (d) $y^+ = 217$; the initial vortex was located at the center of the xz plane.

3.3 Effect of asymmetry

The streamwise alignment of the hairpins is the result of the spanwise symmetric nature of the initial vortex structure. Perfect symmetry however cannot be expected and the hairpins are not usually observed to posses two counter-rotating vortex legs of equal strength. The effect of asymmetry on the initial vortical structure evolution and its development into a hairpin packet has been studied here. Asymmetry was introduced in the initial vortical structure with an asymmetric event in the stochastic estimation procedure. The magnitude of the event vector was kept constant to maintain the initial vortex strength, while the

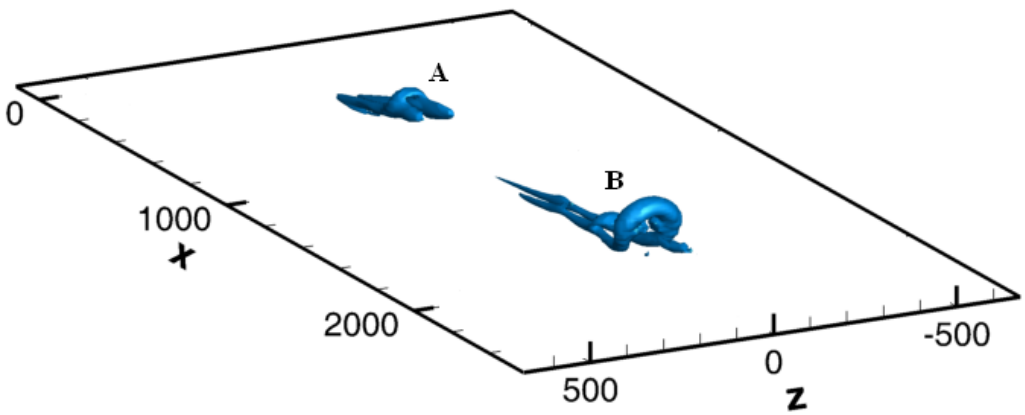
spanwise component of the event vector was increased from zero at the expense of the u and v components. As the β increases, the strength of the event vector is still the same.

$$u = u_m(1-\beta^2)^{1/2} \tag{3.1}$$

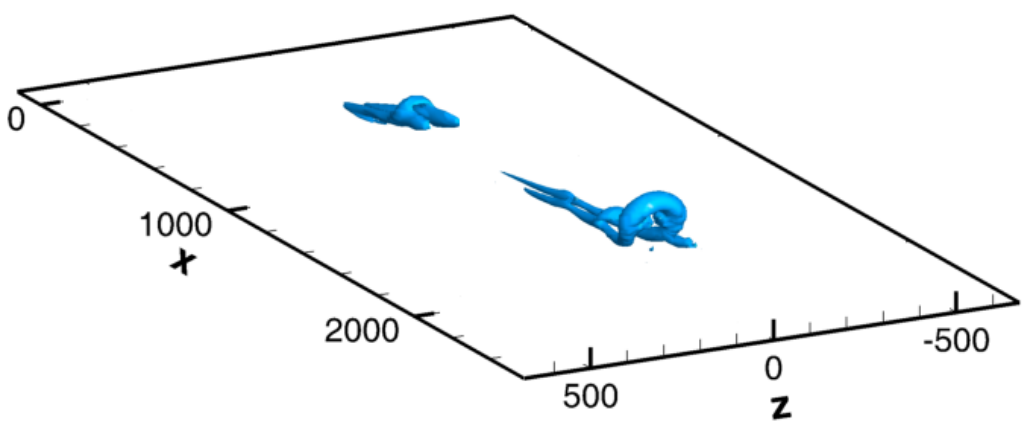
$$v = v_m(1-\beta^2)^{1/2} \tag{3.2}$$

$$w = \beta*(u^2+ v^2)^{1/2} \tag{3.3}$$

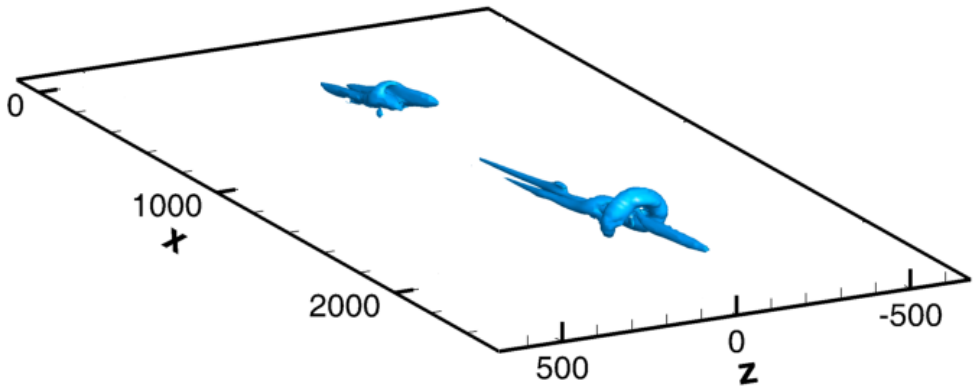
where β is the asymmetry parameter which measures the strength of asymmetry. For β = 0 there is no asymmetry and the initial vortex structure is the same as that shown in figure 6(*a*).



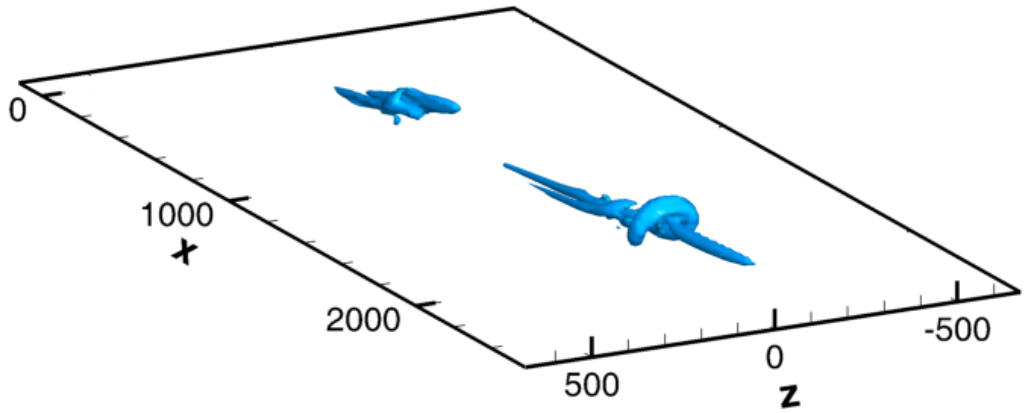
(a)



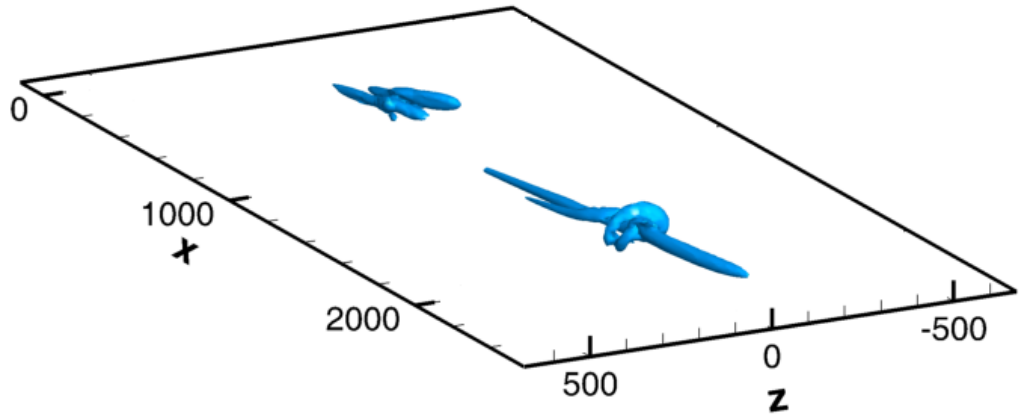
(b)



(c)



(d)



(e)

Figure 3.5 Effect of asymmetry on vortex evolution (a) β = 0.2; (b) β=0.4; (c) β=0.5; (d) β=0.6; (e) β=0.8; α = 2.5 was used for all the computations. The initial field specified was u=(-4,3.5,0) for all the cases considered.

Vortical structure corresponding to an asymmetry parameter of β= 0.2 is initially considered. The resulting initial structure has a pair of quasi-streamwise legs connected by a weak spanwise bridge at the downstream end, but one of the quasi-streamwise legs is much stronger, higher, and longer than the other. The influence of asymmetry on the overall evolution of the hairpin structures remains negligibly small though for β= 0.2. The initial structure has developed into a primary hairpin followed by the generation of secondary and downstream hairpins. The resulting hairpin packet is nearly symmetric and it closely resembles the hairpin packet generated under symmetric initial conditions. Thus, the mechanisms responsible for autogeneration of new hairpin vortices leading to the formation of a hairpin packet remain largely unaffected by small asymmetry in the initial development.

With sufficiently strong asymmetry in the initial event vector, the effects can be distinguished in the initial structure as well as in the evolution. The effects of β=0.4, 0.5, 0.6 and 0.8 are compared.

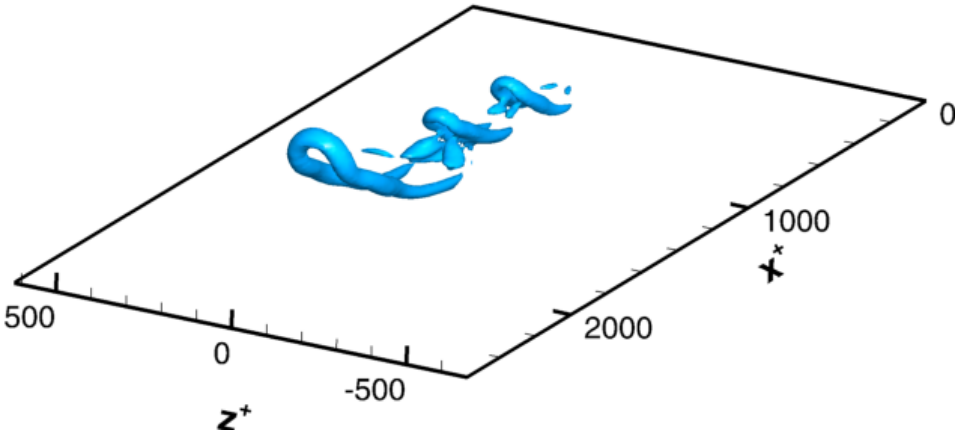
For t^+=150 and beta=0.5, in addition to the primary hairpin, secondary and tertiary hairpin-like structures can also be seen. The right-hand leg of the secondary hairpin can be seen, while the other quasi-streamwise vortex leg is so weak that it is not seen. On the other hand, in the case of the tertiary hairpin only the left-hand quasi-streamwise leg is strong and visible. Therefore, the secondary and tertiary hairpins resemble the asymmetric one-sided cane- or hook-like hairpin vortices referred in literature. Robinson (1991) pointed out that the preferred arrangement for hairpin vortices in a turbulent boundary layer is to be asymmetric and one-

sided. These spanwise asymmetric one-sided hairpins are also known as `canes' [Guezennec & Choi (1989)]. The present results suggest that experimentally observed asymmetry is possibly due to the influence of local spanwise velocity.

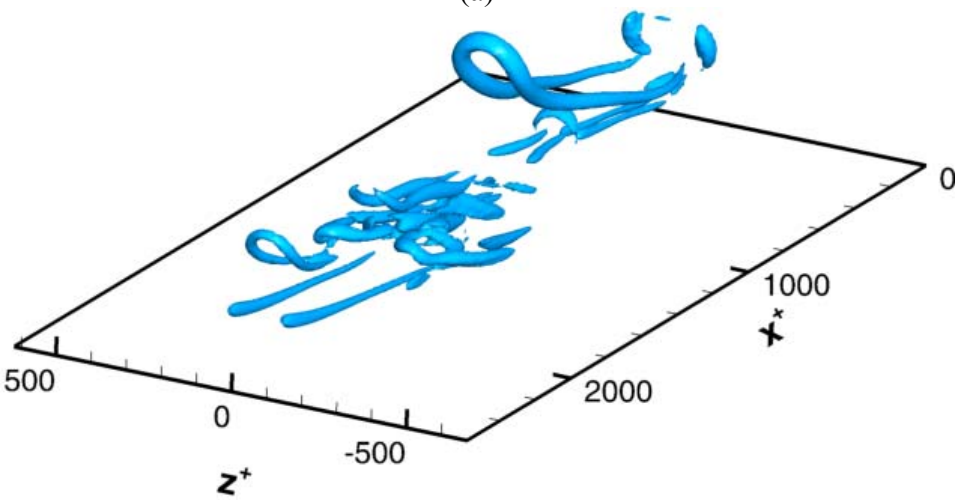
These cane-like secondary and tertiary structures at $t^+ = 150$ are clearly visible in and can be compared with the corresponding symmetric case with initial event vector of $\alpha = 2.5$ specified at $y^+ = 46.6$. For the symmetric case, the streamwise distance between the primary and secondary hairpins was found to be 340 viscous units. In the asymmetric case the streamwise distance between the primary and secondary and between the secondary and tertiary hairpin heads is about 220 and 165 viscous wall units, respectively. These streamwise separations compare better with the experimental measurements of Meinhart, Adrian and Tomkins (1999) who observed the spacing to be around 150 wall units. Furthermore, in the asymmetric case the formation of tertiary hairpin is nearly complete by $t^+ = 150$. In the symmetric case the tertiary hairpin has not even begun to form by this time. In general, it is observed that asymmetry aids in the formation of subsidiary hairpins and the initial threshold amplitude for the formation of secondary and tertiary hairpins is found to be lower with asymmetry. Under asymmetry, the new hairpins form in rapid succession and their streamwise separation is smaller, and hence better compare with the experiments.

3.4 Evolution into a fully turbulent flow

Computations were done to study the vortex evolution into a fully turbulent flow. The linear stochastic estimate at $y^+=46.6$ was used as the initial condition.


0
1000
2000
x^+
500
0
-500
z^+

(a)


0
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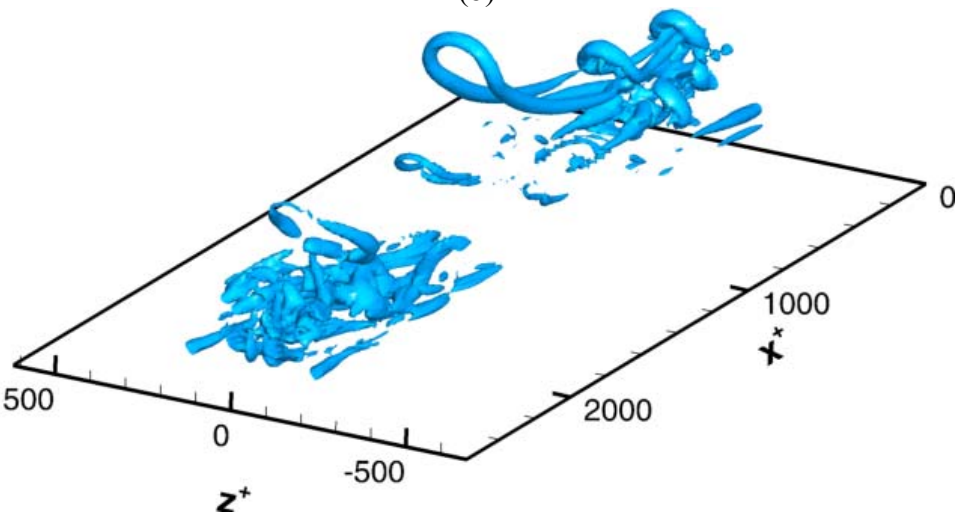
-500
z^+

(b)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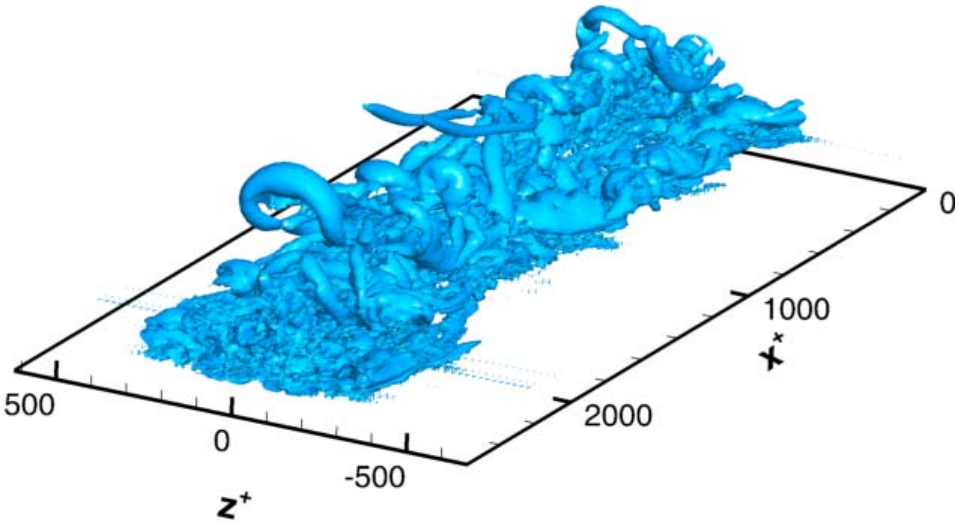
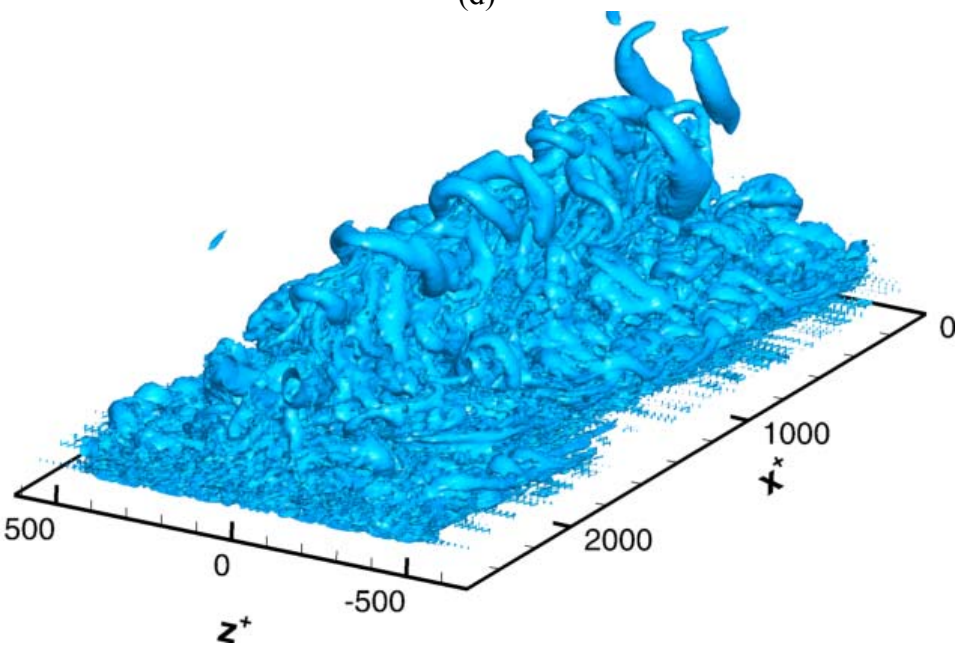
-500
z^+

(c)



(d)



(e)

Figure 3.6 Growth of a single vortex into a fully turbulent field. $\alpha = 2.5$ was used for all the computation. The initial field specified was u=(-4,3.5,0). (a) The evolution at t^+=400; (b) The evolution at t^+=750; (c) The evolution at t^+=1000; (d) The evolution at t^+=1250; (e) The evolution at t^+=1500.

The single vortex at y^+=46.6 auto-generates into the structure in figure 3.6 (a) at t^+=400. These vortices then start growing spanwise apart from growing in height, (figure 3.6 (b)) eventually leading to the complex feature in figure 3.6 (c). This

repeated spanwise interaction and auto-generation results in the structure in figure 3.6 (e) where a chain of vortices on the top is evident. The flow ultimately becomes fully turbulent and occupies the entire channel at around t^+=2000 (figure 3.7).

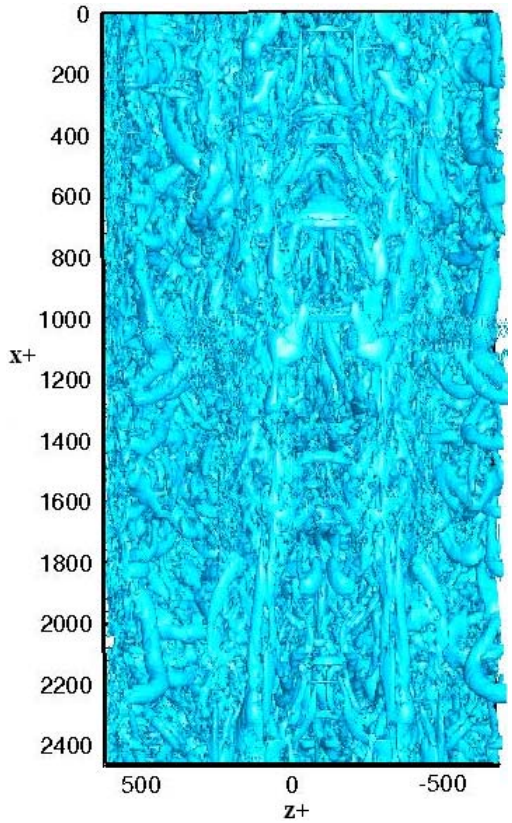


Figure 3.7 Fully turbulent channel flow at t^+=2000.

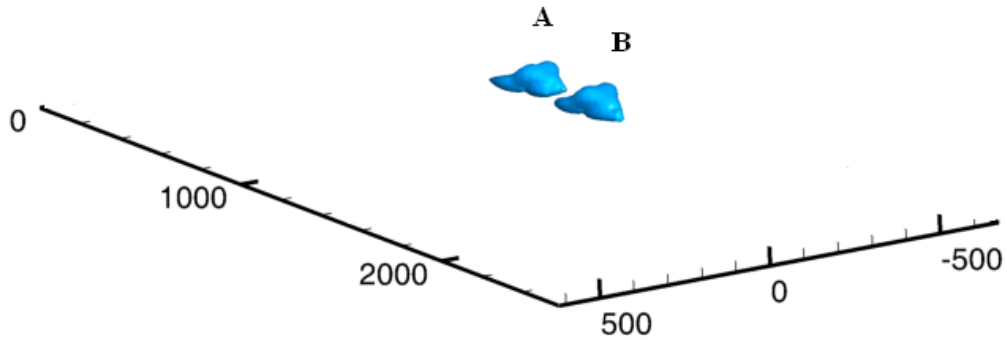
Chapter 4

MULTIPLE VORTEX INTERACTION

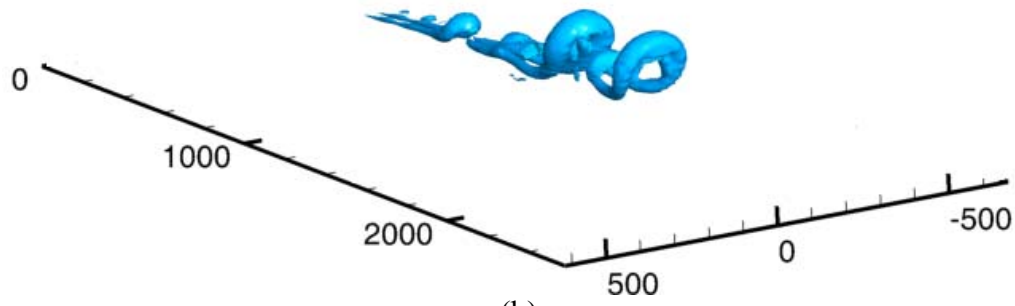
Vortex interactions are important to study since they make understanding on a turbulent field much easier. Since hairpins typically occur in packets, understanding how certain distinct arrangements of vortices evolve helps understand how the entire packet would evolve. In this study, the distinct arrangements like 2 Q2 events, 3 Q2 events and combination of Q2 and Q4 events are studied. Strength plays an important part in this study since the vortices might gain or lose velocity during the process of evolution. Hence, variation of strength for multiple vortex interaction is studied in detail.

4.1 Streamwise interaction between 2 Q2 events

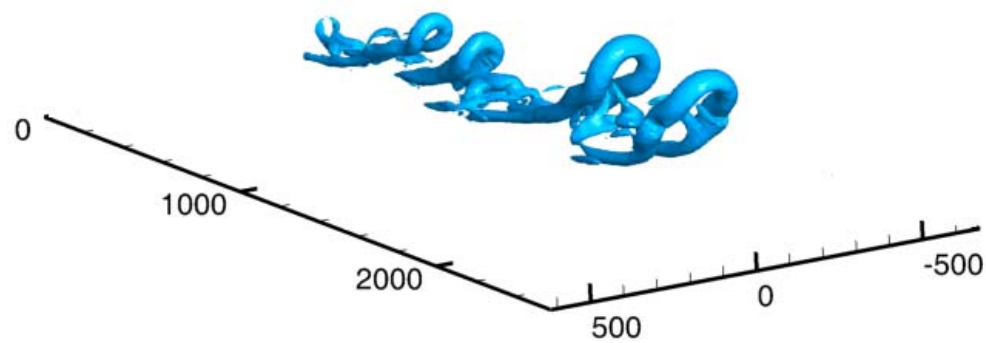
4.1.1 Interaction between 2 Q2 events having the same strength



(a)



(b)

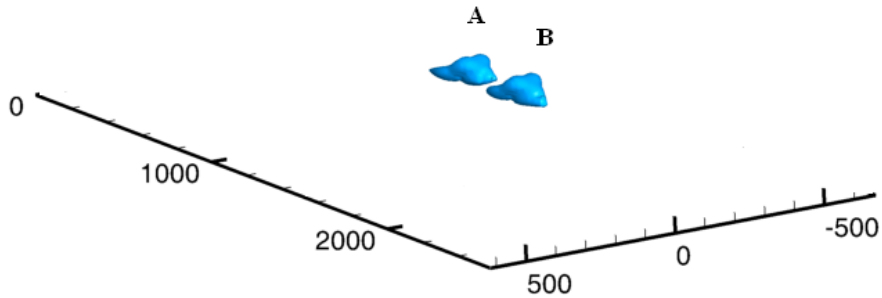


(c)

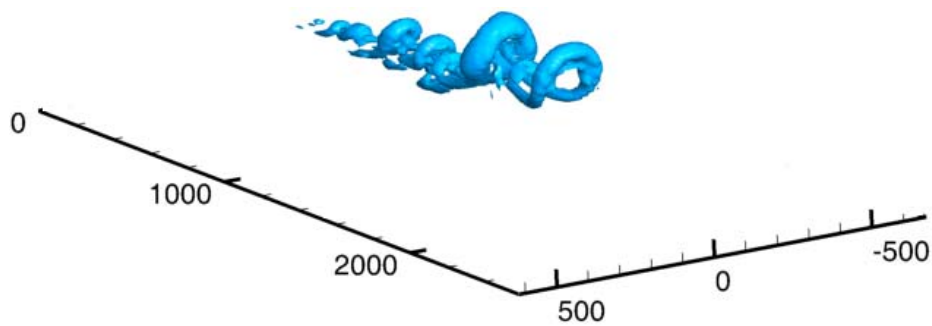
Figure 4.1 Evolution of 2 Q2 events initially separated by x^+ = 100 units. α=2.5; β=0; The initial condition was considered at the center of the xz plane and at y^+=46.6. (a) The initial vortex obtained from linear stochastic estimation. A and B are Q2 events having the initial velocity vectors (-4,3.5,0) based on the joint probability density function (b) The evolution structure at t^+=150 (c) The evolution structure at t^+= 375.

4.1.2 Interaction between 2 Q2 events having the different strengths:

Case I:



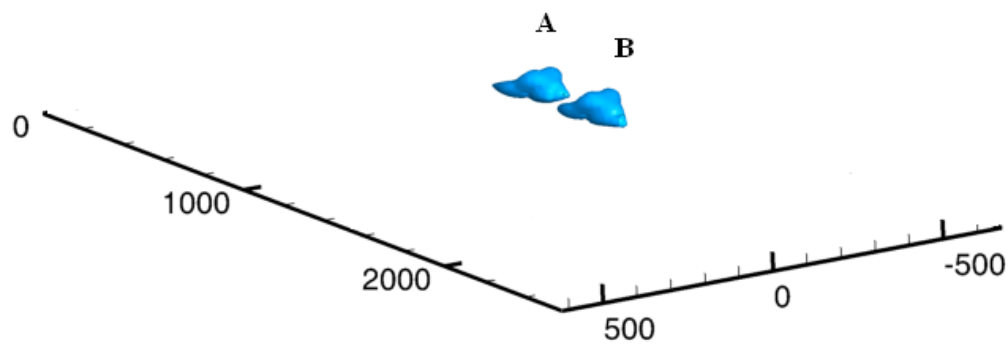
(a)



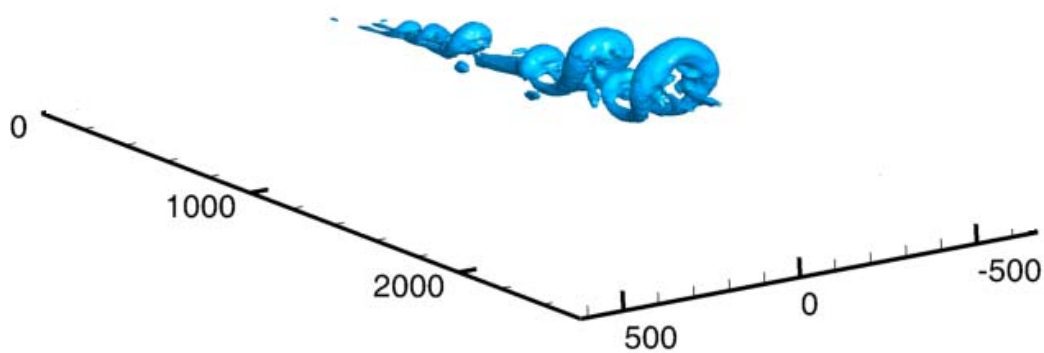
(b)

Figure 4.1 The effect of varying the strength of the vortex. Strength is denoted by α which was defined earlier in the study (chapter 3.1) The vortex A is stronger than vortex B. (a) α_A=2.5; α_B=2; β=0; Hence, the 1st event vector (vortex A) is (-4,3.5,0) and the vortex B event vector is (-3.2,2.8,0) (b) Evolution after t^+= 150

Case II:



(a)



(b)

Figure 4.2 The vortex B is stronger than vortex A. (a) The initial vortex at t^+=0, α_A=2; α_B=2.5; β=0; Hence, event vector for vortex A is (-3.2,2.8,0) and the event vector for vortex B is (-4,3.5,0) (b) Evolution after t^+= 150

A stronger vortex moves slower than the weaker vortex and hence in case I (figure 4.2), the vortices A and B are separated while they evolve. In case II

(figure 4.3) though, vortex A catches up with vortex B and interacts with it earlier than figure 4.2. This can explain the differences in structure at t^+=150 (figures 4.2 (b) and 4.3 (b)). Due to the same reason, the vortex combination in figure 4.2 fills up the length of the channel faster than the weaker-stronger case. It is difficult to quantify the interaction processes due to the non-linearity of the problem.

4.2 Interaction between 3 Q2 events:

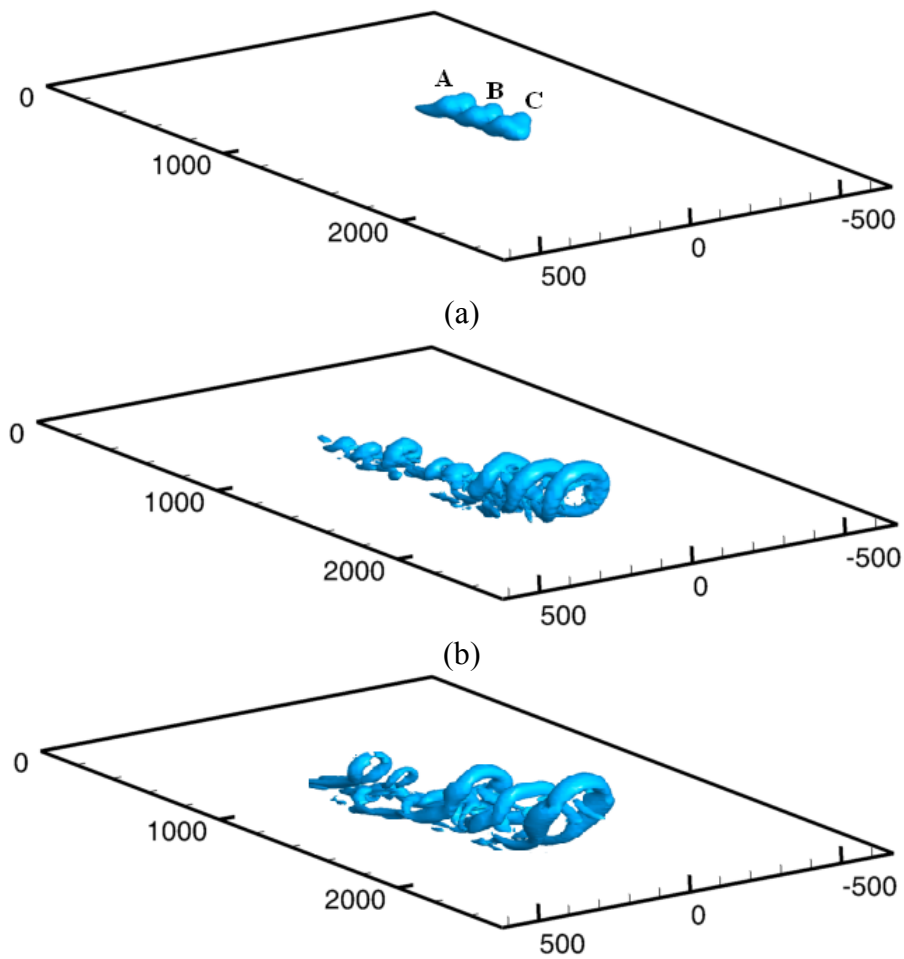
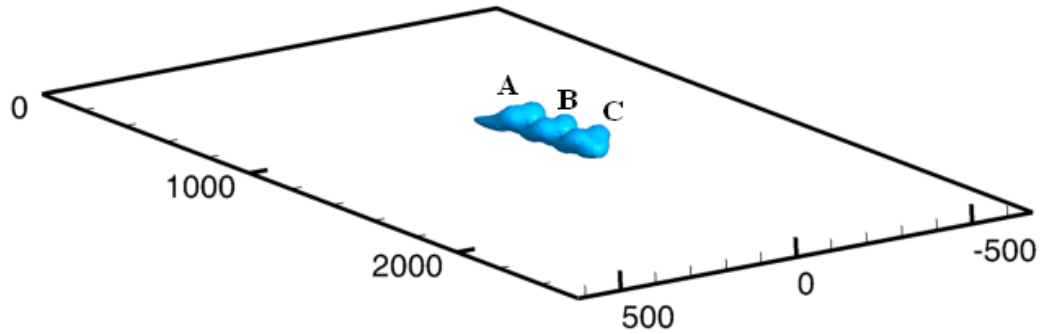
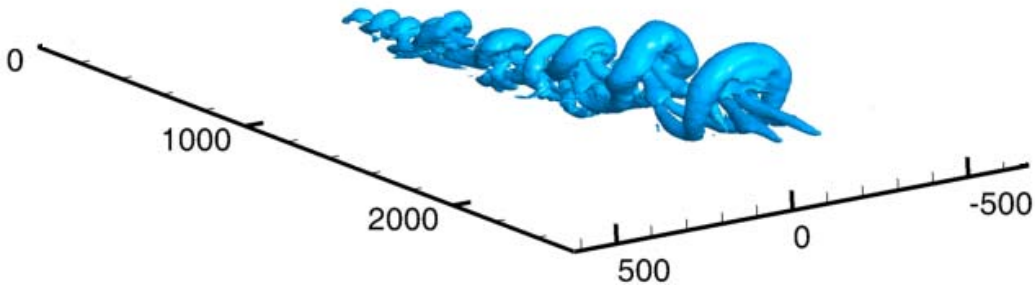


Figure 4.3 Evolution of 3 Q2 events initially separated by x^+ = 100 units. α=2.5; β=0; The initial condition was considered at the center of the xz plane and at y^+=46.6. (a) The initial vortex obtained from linear stochastic estimation (b) The evolution structure at t^+=150 (c) The evolution structure at t^+= 375.

Case I



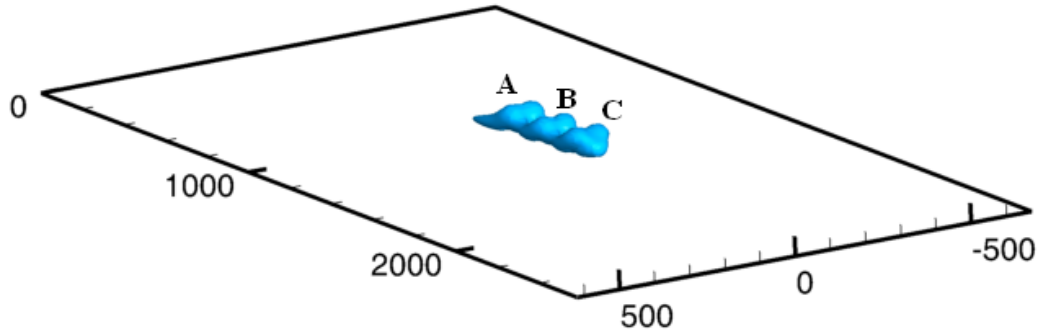
(a)



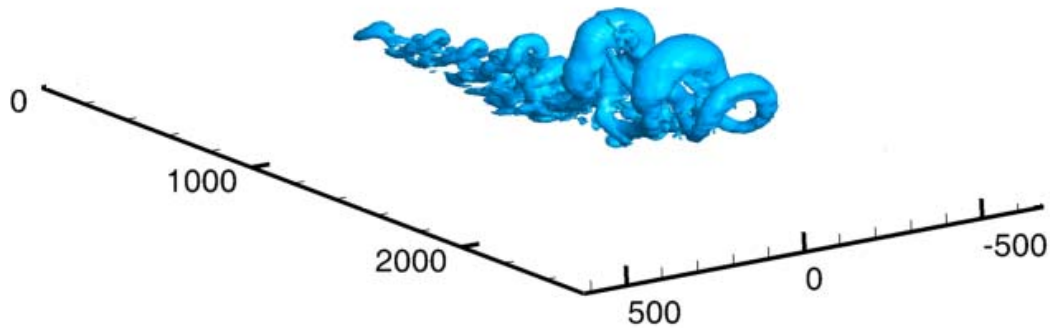
(b)

Figure 4.4 The effect of varying the strength of the vortices. (a) The initial vortex at $t^+=0$. $\alpha_A=3$; $\alpha_B=2.5$; $\alpha_C=2$, $\beta=0$; (b) Evolution after $t^+= 150$

Case II



(a)



(b)

Figure 4.5(a) The initial vortex at $t^+=0$. $\alpha_A=2$; $\alpha_B=2.5$; $\alpha_C=3$, $\beta=0$; (b) Evolution after $t^+= 150$

As explained in section 4.2, the stronger vortex moves slower than the weaker vortex. The interaction can be explained better if the non-linearity in the problem is mathematically modeled.

4.3 Spanwise growth of vortices

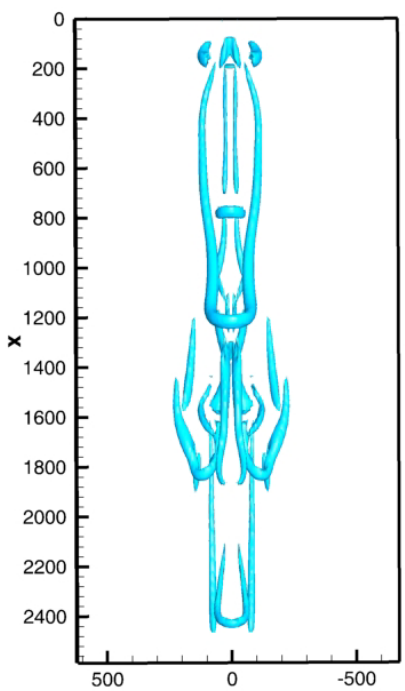
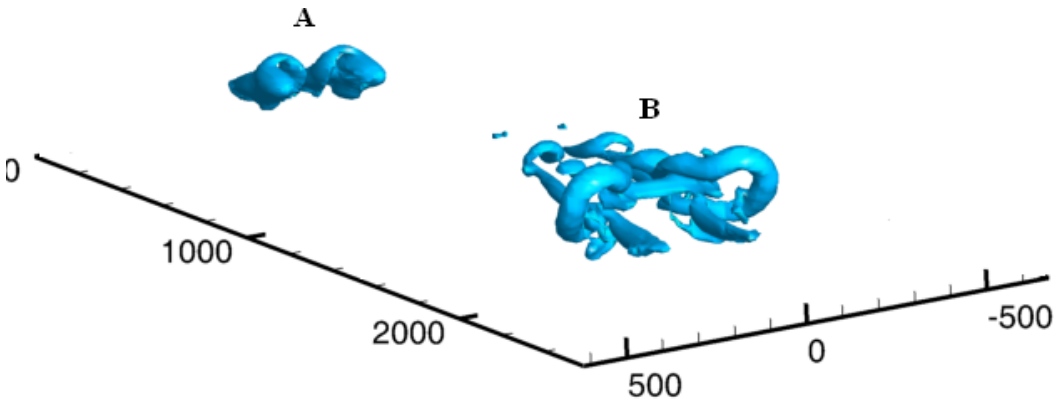
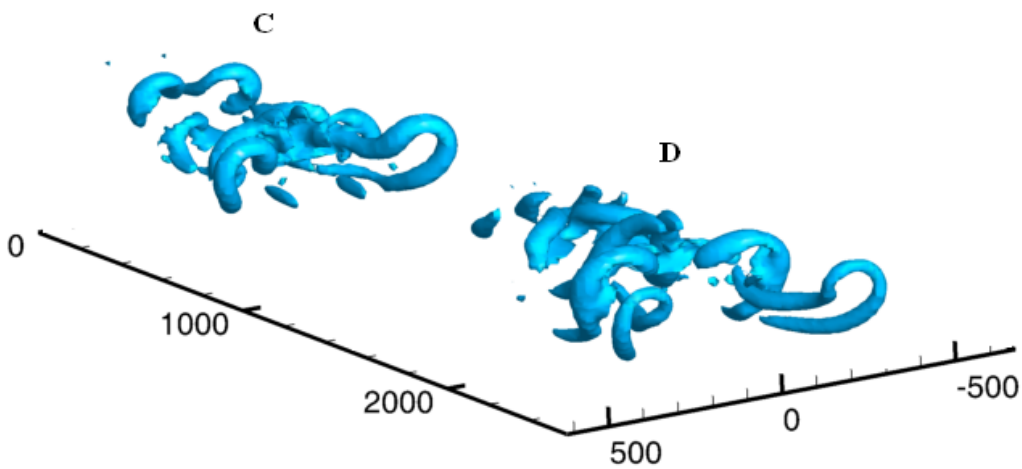


Figure 4.7 The vortex structure at $t^+=750$ for a single Q2 event evolution at ($x^+=0$,$y^+=46.6$, $z^+=0$).

From figure 4.7, it is evident that, as the vortex evolves, it not only generates daughter vortices but also leads to spanwise vortices which interact with each other in a complicated way. This necessitates the study of spanwise vortex interaction.



(a)



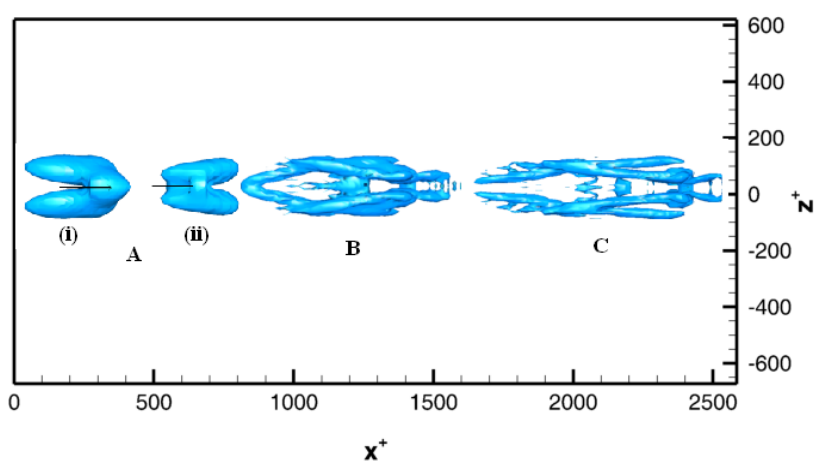
(b)

Figure 4.8 Evolution of 2 spanwise vortices separated by z^+=100 at (a) t^+=25; t^+= 225; (b) t^+=350; t^+=500. Both initial vortices have strength α=2.5 and no inclination to the z axis (β=0).

Lateral interaction between hairpins must be an important ingredient in the spanwise scaling of the hairpin vortices as they grow along the streamwise and wall-normal directions. As the packets expand in the spanwise direction they must ultimately interact by vortex encounters. Encounters also occur due to larger, faster packets running over smaller, slower packets. In lateral encounters, the opposing vorticity in adjacent legs of two hypothetically identical hairpins could annihilate them, resulting in a larger hairpin of the same height, but double the width of the original hairpins. As hypothesized in Adrian, Balachandar and Liu (2001), the merger between 2 spanwise vortices ('A' in figure 4.8 (a)) leads to a larger vortex of the same height ('B' in figure 4.8 (a)). This large vortex auto-generates resulting in asymmetric vortices inclined to the z axis ('C' and 'D' in figure 4.8 (b)).

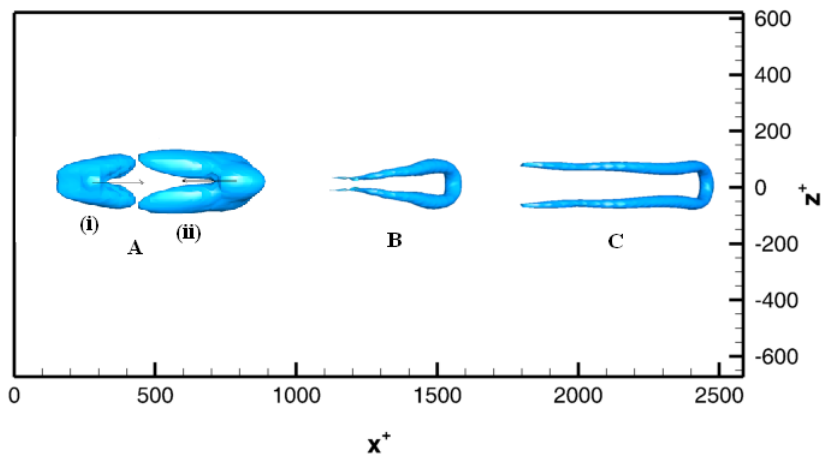
4.4 Interaction between Q2 and Q4 events

Case I



(a)

Case II



(b)

Figure 4.9 Evolution of a Q2 event and a Q4 event together. The vortices are initially separated by x^+ = 100 units. α=2.5; β=0; The initial condition was considered at the center of the xz plane and at y^+=46.6. (a) Q2-Q4 combination where A(i) represents the Q2 vortex and A(ii) represents the Q4 vortex. B represents the structure at t^+=250 and C is the structure at t^+=500 (b) Q4-Q2 combination where A(i) represents the Q4 vortex (4,-3.5,0) at (x^+=0,y^+=46.6, z^+=0, t^+=0) and A(ii) represents the Q2 vortex (-4,3.5,0) at (x^+=100,y^+=46.6, z^+=0, t^+=0). B represents the structure at t^+=250 and C is the structure at t^+=500.

The initial condition in case I grows into a complex structure with the Q4 event developing into 2 quasi-streamwise vortices and the Q2 event auto-generating into daughter vortices although the interaction is non-linear. In case II however, the Q4 vortex rapidly dissipates and a single Q2 hairpin vortex is formed at t^+=250 and t^+=500 (B and C in figure 4.8).

4.5 Interaction between vortices at different y+ locations

Computations were done with 1 vortex at y^+=46.6 and the other at y^+=11.8 separated by x^+=100 units. The higher vortex consumes the lower one at a very early time (t^+=50) and the combination behaves similar to the single vortex evolution (figure 4.11).

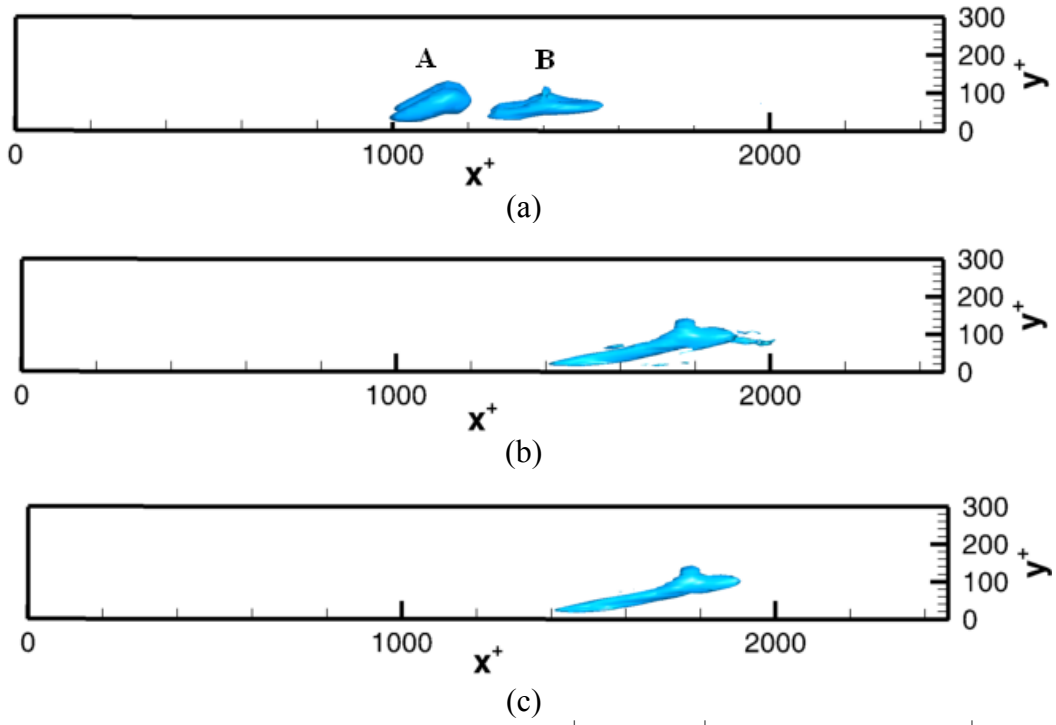


Figure 4.10 (a) 2 vortices separated by 100 x^+ units at t^+=0. Vortex A is at y^+=46.6 and vortex B is at y^+=11.8; (b) the vortex structure at t^+=50; (c) The vortex structure at t^+=50 when the vortex B is absent;

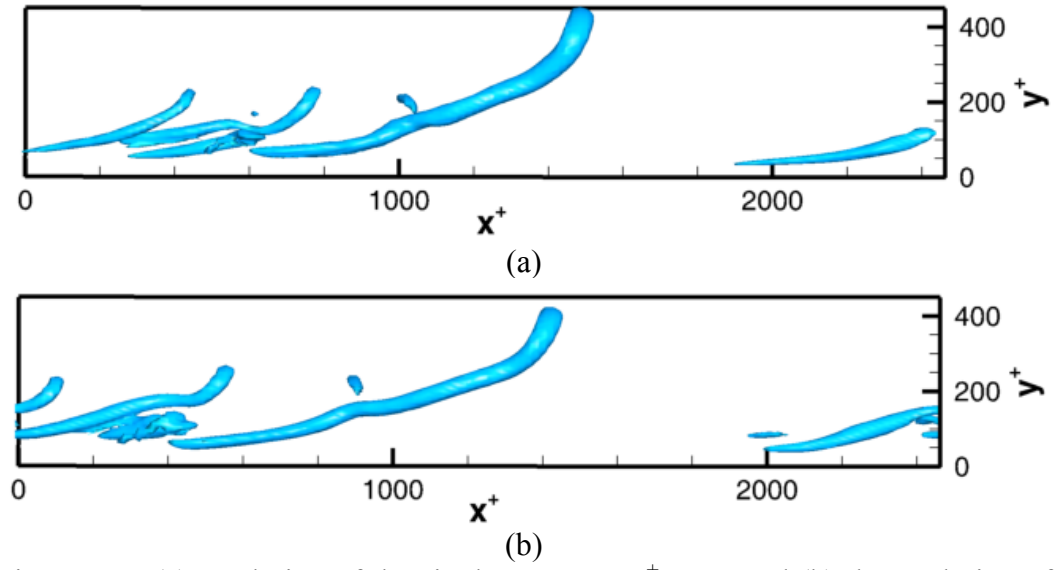
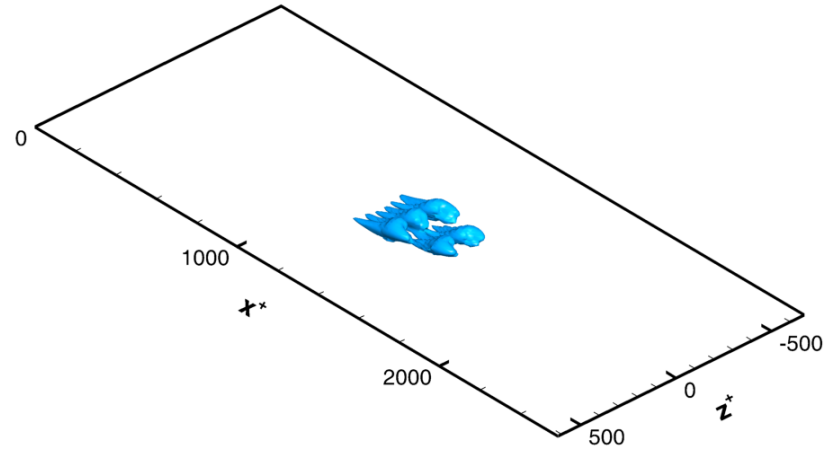
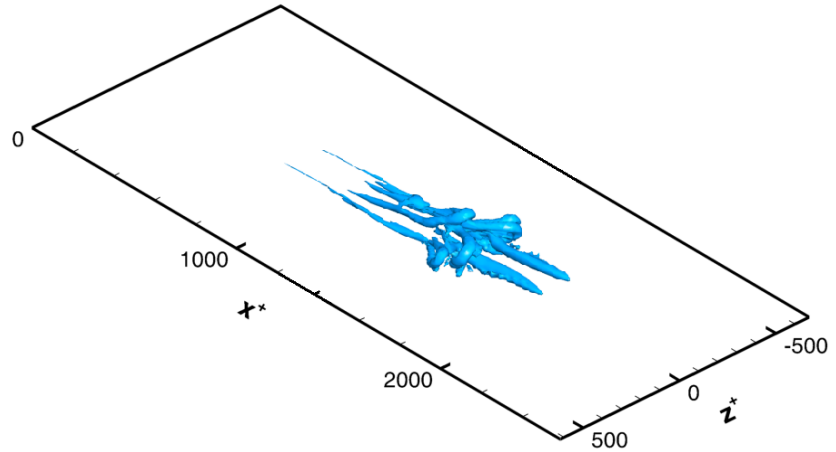


Figure 4.11 (a) Evolution of the single vortex at y^+=46.6 and (b) the evolution of the dual vortices at t^+ = 400. The similarity in structure leads us to believe that vortex B doesn't have a major role to play in the evolution.

4.6 Interaction between vortices in a staggered arrangement



(a)



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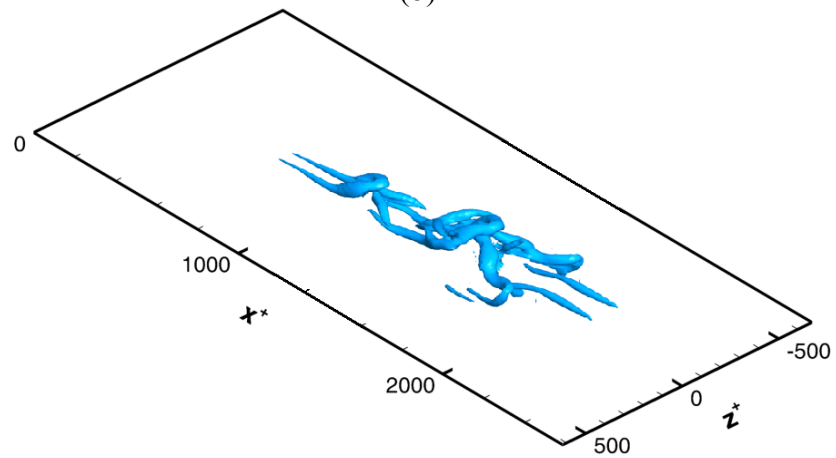
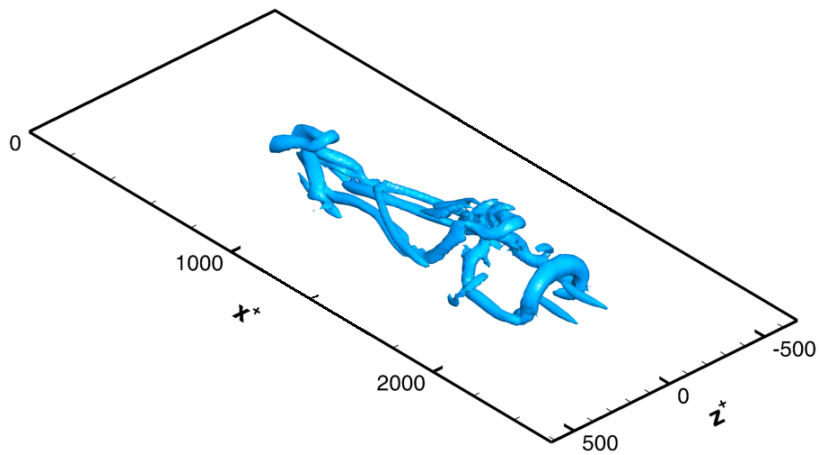


(c)



(d)

Figure 4.12 Evolution of 5 Q2 events placed in a staggered arrangement. The schematic diagram of the arrangement is shown in figure 4.13.α=2.5; β=0; All the initial vortices are at y^+=46.6. (a) The evolution structure at t^+=25 (b) The evolution structure at t^+=175 (c) The evolution structure at t^+= 375 (d) The evolution structure at t^+=500.

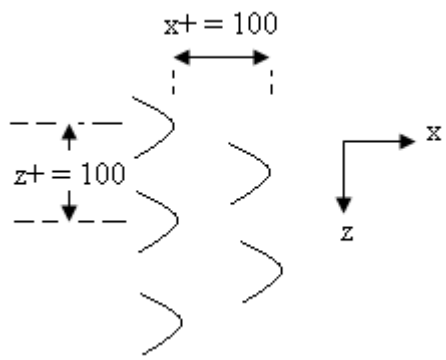


Figure 4.13 A schematic arrangement of staggered vortices in channel flow

The vortices in figure 4.12 (a) grow asymmetrically (with inclination to the z axis) till t^+=175. The canes formed in figure 4.12 (b) then dissipate leading to the vortex structure in figure 4.12 (d). After t^+=175, there is no more cane formation.

Chapter 5

CONCLUSIONS AND RECOMMENDATIONS

This study attempted to answer questions concerning how vortex mergers produce larger scale structures, a process that may contribute to the growth of length scale with increasing distance from the wall in turbulent wall flows. This would aid in modeling the von Karman constant which is crucial in drag related studies.

The dynamics of hairpin vortices in turbulent channel flow have been studied using direct numerical simulation. The two-point spatial correlation of the fully turbulent velocity field was initially studied in detail and compared to existing literature. Linear stochastic estimation was then used to estimate the structures of the initial three-dimensional vortices. The vortices were visualized using the iso-surface of the imaginary part of the conjugated complex eigen values of the local velocity gradient tensor (λ_{ci}). The Reynolds number of the present simulation is more than twice that of the Re_τ=180 flow studied by Zhou et al. (1999), and a number of new types of events such as quasi-streamwise vorticity and Q4 events were studied in this work. The larger Re_τ also made it possible to simulate the evolution of the vortices over longer periods of time, and correspondingly larger head heights.

The effect of asymmetry, y^+ position and strength were evaluated for single vortices. In order to study the complex non-linear interactions between vortices, various parameters such as spanwise inclination and strength were varied.

Grid independence study was performed to choose the optimum grid. The following are the conclusions from this study.

1. Autogeneration is insensitive to Re_τ, as results change little from Re_τ=180 (Zhou et al. 1999) to Re_τ=395. The forms of the eddies at Re_τ=395 are similar to those at Re_τ=180, although there is no auto-generation evident upto α=1.25. Hence, the auto-generation threshold is shifted from α=1 for Re_τ=180 to α=1.25 for Re_τ=395.
2. Single vortex evolution: Just like the strength threshold for auto-generation, there exists asymmetry threshold for cane formation. Canes are not produced till β=0.4. For a symmetric evolution, the flow becomes fully turbulent and occupies the entire channel around t^+=2000.
3. Multiple vortex interaction
    a. Larger Q2 overtakes smaller Q2
    b. Smaller Q2 behind a larger Q2 just separates.
    c. Q2 behind Q4 leads to auto-generation with the Q4 event becoming 2 quasi-streamwise vortices at t^+=500.
    d. Q4 behind Q2 rapidly dissipates the Q4 vortex.
    e. Lateral vortices merge in t^+=100.
    f. Staggered vortices merge in t^+=175.
    g. Two vortices, one at y^+=46.6 and the other at y^+=11.8, separated by x^+=100 evolve in a similar fashion to a single vortex at y^+=46.6; i.e. the vortex at a lower y^+ value does not play a significant part in the evolution.

Future work would include specifying $\mathbf{d}(\mathbf{x},t)$ in addition to $\mathbf{u}(\mathbf{x},t)$ which would lead to a more detailed picture. The full potential of stochastic estimation is realized when all the components of the given data $\mathbf{u}(\mathbf{x},t)$ and possibly $\mathbf{d}(\mathbf{x},t)$ are specified. Attempts also need to be made to separate the linear and non-linear effects to simplify the problem. Higher Reynolds numbers and bigger domains (eg. doubling the length of the channel) are recommended based on the computational resources available.

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APPENDIX A

LINEAR STOCHASTIC ESTIMATION DERIVATION

Let g(x') be any quantity associated with the turbulent flow, and let $E_1(x_1)$, $E_2(x_2)$, $E_3(x_3)$,…, $E_N(x_N)$ be N random whose value assume specified event values at (possibly) N different points. The conditionally averaged flow field is the averaged flow field given that the specified events occur [Zhou et. al. (1999)]:

$$<g(x')|E_1(x_1), E_2(x_2), E_3(x_3),\ldots, E_N(x_N)> \quad \text{(A1)}$$

It is the best estimate of the flow field in terms of the known event , in the mean square sense.. To streamline the nottion, we often let **E** be the N dimensional event vector

$$\mathbf{E}=[\ f_1 \leq E_1(\mathbf{x}_1) < f_1+d\ f_1 \text{ and } \ldots \text{ and } f_N \leq E_N(\mathbf{x}_N) < f_N+df_N] \quad \text{(A2)}$$

The *linear stochastic estimate* of a conditional average is found by expanding the conditional average in a power series about the event E =0, and truncating the expansion at some level,

$$<g_i|E>=L_{il}E_l+N_{ilm}E_lE_m+\ldots \quad \text{(A3)}$$

The unknown coefficients **L** , **N** etc. are determined by requiring that the mean-square error between the approximation and the conditional average be minimized.
In the case of linear estimation only the first term is retained and the minimization leads to a set of linear algebraic equations for L_{il},

$$<E_m(x_m)E_l(x_m)>\ L_{il} = E_m(x_m)\ g_i(x')> \quad \text{(A4)}$$

Where l=1,2,3,...,N and m=1,2,3...,N.We assume that the event and the estimated quantity have zero mean in equations (A3) and (A4).

Equation (A4) can be written as

$$AL_i = b_i \quad \text{(A5)}$$

Since the streamwise (x) and spanwise (z) directions are homogenous in the periodic channel flow,

$$A_{ml} = R_{EmEl}(x_l-x_m,\ y_m,\ z_l-z_m) \quad \text{(A6)}$$

and

$$b_{im} = R_{Emgl}(x'-x_m,\ y_m, y',\ z'-z_m) \quad \text{(A7)}$$

L_i can be obtained from solving the matrix equation with N x N symmetric coefficient matrix A. Finally, the linear stochastic estimation (LSE) of the conditional average is

$$<g_i|E> \sim L_{il}(x';x_1,\ x_2,\ \ldots,\ x_N)E_l(x_l) \quad \text{(A8)}$$

$$L_{il} = \begin{bmatrix} < u_1 u_1 > < u_2 u_1 > < u_3 u_1 > \\ < u_1 u_2 > < u_2 u_2 > < u_3 u_2 > \\ < u_1 u_3 > < u_2 u_3 > < u_3 u_3 > \end{bmatrix} \tag{A9}$$

APPENDIX B

LINEAR STOCHASTIC ESTIMATION CODE

This code uses correlation functions to produce a conditional vortex using linear stochastic estimation.

Grid:128 x 129 x 128;

Re_τ=395;

Language: Fortran 95;

Machine it ran on: Saguaro (ASU high performance computing center);

Number of processors: 1;

Input parameters: u,v and w components of velocity, strength α, asymmetric factor β, position y^+;

Output parameters: up.dat, vp.dat, wp.dat (velocity fields in .dat format), l_ci.dat (λ_{ci} in .dat format)

```
      include 'param.h'
      common/LSE/nv_evn(N_evn),nv_est(N_est),multi(N_evn,3),j1
      common/domain/sx,sz
      common/para/re

      real*8 event(N_evn)
      real*8 AI(N_evn,N_evn)

      real*8 b(N_evn,nx,nyp,nz)
      real*8 CL(N_evn,nx,nyp,nz)
      character*8 dummy8
      character*45 dummy45

      re =  395.

      Pi = acos(-1.0)
      sx = 2. * pi
      sz = 1./1. * pi

      open(70,file='lse.set',status='old',action='read')
      read(70,102) dummy45
      write(*,102) dummy45
      read(70,100) dummy8,alpha
      write(*,100) dummy8,alpha
      read(70,100) dummy8,beta
      write(*,100) dummy8,beta
100   format(a8,e14.8)
101   format(a8,i5)
```

```
102   format(a45)


      call setup

c---  set event or condition variables and locations

      nv_evn(1) = 1   ! u'
      nv_evn(2) = 2   ! v'
      nv_evn(3) = 3   ! u'
c      nv_evn(4) = 1   ! u'
c      nv_evn(5) = 2
c      nv_evn(6) = 3
c      nv_evn(7) = 1
c       nv_evn(8) = 2
c      nv_evn(9) = 3
c      nv_evn(10) = 1
c      nv_evn(11) = 2
c      nv_evn(12) = 3
c      nv_evn(13) = 1
c      nv_evn(14) = 2
c      nv_evn(15) = 3

      event(:)= 0.0

      read(70,102) dummy45
      write(*,102) dummy45
      read(70,101) dummy8,j1
      write(*,101) dummy8,j1

c---  event variables are normalized by wall units

      do ll=1,N_evn
         read(70,103) dummy8,event(ll),(multi(ll,k),k=1,3)
         write(*,103) dummy8,event(ll),(multi(ll,k),k=1,3)
103      format(a8,e12.5,3i3)
      enddo

c--- for multi location event  -> Read from lse.set file
c         multi(ll,1)   ! relative x location of ll-th event w.r.t 1st
event location
c         multi(ll,2)   ! relative y location of ll-th event w.r.t 1st
event location
c         multi(ll,3)   ! relative z location of ll-th event w.r.t 1st
event location
c---
c–impose asymmetry in z dir.
      Event(3) = beta*(event(1)**2 + event(2)**2)**0.5  ! w_m=
(u_m^2+v_m^2)^0.5
      event(1) = event(1)*(1.0-beta**2)**0.5
      event(2) = event(2)*(1.0-beta**2)**0.5

c--- multiply strength factor to event vector
      event = alpha*event
```

```
      do ll=1,N_evn
         write(*,104) ll,event(ll),(multi(ll,k),k=1,3)
104      format(i5,e12.5,3i3)
      enddo


c---  set the quantities which will be estimated by LSE

      nv_est(1) = 1 ! u'
      nv_est(2) = 2 ! v'
      nv_est(3) = 3 ! w'

c----

      call set_coef_AI(AI)  ! AI = inverse of A

      do i_est = 1, N_est

         call read_b(b,i_est)
         call get_CL(CL,AI,b)
         call do_LSE(CL,event,i_est)

      enddo  ! N_est

      call out_put(event)


      stop
      end

c----+-------------------------------------------------------
      subroutine setup
      include 'param.h'
      common/mesh/y(nyp),dx,dz
      common/domain/sx,sz

      pi = acos(-1.0)

      do j=1,nyp
         y(j)=1.-cos(pi*real(j-1)/real(nyp-1))
      enddo

      dx = sx/real(nx)
      dz = sz/real(nz)

      return
      end

c----+-------------------------------------------------------
      subroutine set_coef_AI(AI)

      include 'param.h'
      common/LSE/nv_evn(N_evn),nv_est(N_est),multi(N_evn,3),j1

      real*8 r(N_evn),x(N_evn)
```

```
      real*8 A(N_evn,N_evn)
      real*8 AI(N_evn,N_evn)
      real*8  test(N_evn,N_evn)

      character*50 filename
      real*8 E(N_evn,nx,nyp,nz)
      real*8 Em(N_evn),Eq(N_evn,N_evn)

      real*8 t(nx,nyp,nz)

      A(:,:)  = 0.0
      AI(:,:)= 0.0

c---

      do m=1,N_evn
         do l=m,N_evn

         i_m = multi(m,1)
         j_m = j1 + multi(m,2)
         k_m = multi(m,3)
         i_l = multi(l,1)
         j_l = j1 + multi(l,2)
         k_l = multi(l,3)

         filename = '../03_corr/R_'
         nn=index(filename,'R')
         write(unit=filename(nn+2:),fmt='(bn,i2.2)') nv_evn(m)
         write(unit=filename(nn+4:),fmt='(bn,a1)')   '_'
         write(unit=filename(nn+5:),fmt='(bn,i2.2)') nv_evn(l)
         write(unit=filename(nn+7:),fmt='(bn,a2)')   'Y_'
         write(unit=filename(nn+9:),fmt='(bn,i3.3)') j_m
         write(*,*) filename

         open(10,file=filename,form='unformatted')
         read(10) (((t(I,j,k),i=1,nx),j=1,nyp),k=1,nz)
         close(10)

         A(m,l) = t(nx/2+i_l-i_m,j_l,nz/2+k_l-k_m)

         enddo
      enddo

c----

c---  A(m,l) should be symmetric.

      Do m=2,N_evn
         do l=1,m-1
            A(m,l)=A(l,m)
         enddo
      enddo

c---  calculate the inverse of A
```

```
      call FindInv(A, AI, N_evn, ErrorFlag)

c--- check inversion of A
      test = 0.0
      do j=1, N_evn
      do i=1, N_evn
         do m=1,N_evn
            test(I,j) = test(I,j) + A(I,m)*AI(m,j)
         enddo
      enddo
      enddo

         write(*,*) 'check the inversion'
      do I = 1, N_evn
         write(*,*) (test(I,j),j=1,N_evn)
      enddo

c---

c      do m=1,N_evn
c         write(*,100) (A(m,l),l=1,N_evn)
c      enddo
c         write(*,*)
c      do m=1,N_evn
c         write(*,100) (AI(m,l),l=1,N_evn)
c      enddo
c100   format(4(E12.5,x))

      return
      end

c----+-------------------------------------------------------
      subroutine read_b(b,i_est)

      include 'param.h'
      common/LSE/nv_evn(N_evn),nv_est(N_est),multi(N_evn,3),j1

      real*8 t(N_evn,nx,nyp,nz)
      real*8 b(N_evn,nx,nyp,nz)

      character*50 filename

      do m = 1, N_evn

        j_m = j1 + multi(m,2)
c         j_m = j1

         filename = '../03_corr/R_'
         nn=index(filename,'R')
         write(unit=filename(nn+2:),fmt='(bn,i2.2)') nv_evn(m)
         write(unit=filename(nn+4:),fmt='(bn,a1)')   '_'
         write(unit=filename(nn+5:),fmt='(bn,i2.2)') nv_est(i_est)
         write(unit=filename(nn+7:),fmt='(bn,a2)')   'Y_'
         write(unit=filename(nn+9:),fmt='(bn,i3.3)') j_m
         write(*,*) filename
```

```
         open(10,file=filename,form='unformatted')
         read(10) (((t(m,I,j,k),i=1,nx),j=1,nyp),k=1,nz)
         close(10)

         do j=1,nyp
            do k=1,nz
            do i=1,nx

               i_m = i - multi(m,1)
               k_m = k - multi(m,3)
               if (i_m.lt.1) i_m = i_m + nx
               if (k_m.lt.1) k_m = k_m + nz

               b(m,I,j,k) = t(m,i_m,j,k_m)

            enddo
            enddo
         enddo

      enddo

      return
      end

c----+-------------------------------------------------------
      subroutine get_CL(CL,AI,b)

      include 'param.h'
      common/LSE/nv_evn(N_evn),nv_est(N_est),multi(N_evn,3),j1

      real*8 AI(N_evn,N_evn)

      real*8 b(N_evn,nx,nyp,nz)
      real*8 CL(N_evn,nx,nyp,nz)

      CL(:,:,:,:)= 0.0

      do l=1,N_evn
         do k=1,nz
         do j=1,nyp
         do i=1,nx
            do m=1,N_evn
               CL(l,i,j,k)=CL(l,i,j,k)+AI(l,m)*b(m,i,j,k)
            enddo
         enddo
         enddo
         enddo
      enddo

      return
      end

c----+-------------------------------------------------------
      subroutine do_LSE(CL,event,i_est)
```

```
      include 'param.h'
      common/LSE/nv_evn(N_evn),nv_est(N_est),multi(N_evn,3),j1
      common/domain/sx,sz
      common/mesh/y(nyp),dx,dz

      real*8 event(N_evn)
      real*8 CL(N_evn,nx,nyp,nz)

      real*8 g(nx,nyp,nz) ! estimated quantity

      character*50 filename

      g(:,:,:) = 0.0

      do k=1,nz
      do j=1,nyp
      do i=1,nx
         do l=1,N_evn
            g(I,j,k) = g(I,j,k) + CL(l,I,j,k)*event(l)
         enddo
      enddo
      enddo
      enddo

      filename = 'output_LSE'
      nn=index(filename,'E')
      write(unit=filename(nn+1:),fmt='(bn,i1.1)') i_est
      write(*,*) filename
      open(10,file=filename,status='unknown',form='unformatted')
      write(10) (((g(I,j,k),i=1,nx),j=1,nyp),k=1,nz)
      close(10)

      return
      end

c----+-------------------------------------------------------
      subroutine out_put(event)

      include 'param.h'
      common/LSE/nv_evn(N_evn),nv_est(N_est),multi(N_evn,3),j1
      common/mesh/y(nyp),dx,dz
      common/domain/sx,sz
      common/para/re

      real*8 event(N_evn)

      real*8 g(N_est,nx,nyp,nz)
               ! -> usually N_est=1,2,3 denote u,v,w

      real*8 um(nyp)

      character*50 filename

      real*8 l_ci(nx,nyp,nz)
```

```
c---  read the estimated field from file

      g(:,:,:,:) = 0.0

      do i_est=1,N_est
         filename = 'output_LSE'
         nn=index(filename,'E')
         write(unit=filename(nn+1:),fmt='(bn,i1.1)') i_est
         write(*,*) filename
         open(10,file=filename,status='unknown',form='unformatted')
         read(10) (((g(i_est,I,j,k),i=1,nx),j=1,nyp),k=1,nz)
         close(10)
      enddo

c---  read averaged statistics
      open(10,file='../01_mean/output.dat',status='old')
      do j=1,nyp
         read(10,200)
     &   dummy,um(j),dummy,dummy,dummy,dummy,dummy,
     &   dummy,dummy,dummy,dummy,dummy,dummy
      enddo
200   format(13(e12.5,x))
      close(10)


c--- total velocity

      do k=1,nz
      do j=1,nyp
      do i=1,nx
         g(1,i,j,k) = g(1,i,j,k)+um(j)
      enddo
      enddo
      enddo

c--- write estimated velocity field

      open(10,file='u.dat',status='unknown',form='unformatted')
      write(10) (((g(1,I,j,k),i=1,nx),j=1,nyp),k=1,nz)
      close(10)

      open(10,file='v.dat',status='unknown',form='unformatted')
      write(10) (((g(2,I,j,k),i=1,nx),j=1,nyp),k=1,nz)
      close(10)

      open(10,file='w.dat',status='unknown',form='unformatted')
      write(10) (((g(3,I,j,k),i=1,nx),j=1,nyp),k=1,nz)
      close(10)

c---  calculate lambda_ci

      call get_lambda_ci(g,l_ci)

      open(11,file='l_ci.dat',status='unknown')
```

```
      write(11,*) “variables=x,y,z,lci,u,v,w,uf”
      write(11,*)
     >’zone i=’,nx/3*2-nx/3+1,’, j=’,nyp,’,k=’,nz/3*2-nz/3+1,’,f=point’

      do k=nz/3,nz/3*2
      do j=1,nyp
      do i=nx/3,nx/3*2
         yy=y(j)*re
         xx=real(i-1)*dx*re
         zz=real(k-1)*dz*re
         write(11,102) xx,yy,zz,l_ci(I,j,k)
     >                ,(g(m,I,j,k),m=1,3)
     >                , g(1,i,j,k)-um(j)
102      format(8(e12.5,x))
      enddo
      enddo
      enddo
      close(11)

      return
      end


c----+-------------------------------------------------------
      subroutine get_lambda_ci(g,l_ci)

      include ‘param.h’
      common/mesh/y(nyp),dx,dz
      common/domain/sx,sz
      common/para/re

      real*8 g(3,nx,nyp,nz)
               !-> 1,2,3 denote u,v,w

      real*8 l_ci(nx,nyp,nz)

      real*8 d11(nx,nyp,nz),d12(nx,nyp,nz),d13(nx,nyp,nz)
      real*8 d21(nx,nyp,nz),d22(nx,nyp,nz),d23(nx,nyp,nz)
      real*8 d31(nx,nyp,nz),d32(nx,nyp,nz),d33(nx,nyp,nz)

      real*8 q1(nx,nyp,nz)
      real*8 q2(nx,nyp,nz)
      real*8 q3(nx,nyp,nz)

c--- d_ij = dq_i/dx_j

      call init_partial
      call fftw_ini

      do k=1,nz
      do j=1,nyp
      do i=1,nx
         q1(I,j,k) = g(1,I,j,k)
      enddo
      enddo
```

```
      enddo

      call partial(1,q1,d11)
      call partial(2,q1,d12)
      call partial(3,q1,d13)

      do k=1,nz
      do j=1,nyp
      do i=1,nx
         q2(I,j,k) = g(2,I,j,k)
      enddo
      enddo
      enddo

      call partial(1,q2,d21)
      call partial(2,q2,d22)
      call partial(3,q2,d23)

      do k=1,nz
      do j=1,nyp
      do i=1,nx
         q3(I,j,k) = g(3,I,j,k)
      enddo
      enddo
      enddo

      call partial(1,q3,d31)
      call partial(2,q3,d32)
      call partial(3,q3,d33)


c---  calculating lambda_ci

      l_ci(:,:,:) = 0.0d0 ! l_ci

      do 1 j=1,nyp
      do 1 k=1,nz
      do 1 i=1,nx
         e11 = d11(i,j,k)
         e12 = d12(i,j,k)
         e13 = d13(i,j,k)
         e21 = d21(i,j,k)
         e22 = d22(i,j,k)
         e23 = d23(i,j,k)
         e31 = d31(i,j,k)
         e32 = d32(i,j,k)
         e33 = d33(i,j,k)
         p = - (e11 + e22 + e33)
         q = 0.5*(p**2 – (
     &                  +e11**2
     &                  +e22**2
     &                  +e33**2
     &                  +e12*e21*2.0
     &                  +e13*e31*2.0
     &                  +e23*e32*2.0
```

```
     &                    )
     &              )
         r = -( - e13*e22*e31 + e12*e23*e31
     &          + e13*e21*e32 – e11*e23*e32
     &          - e12*e21*e33 + e11*e22*e33
     &         )

         r0 = r + 2./27.*p**3 – 1./3.*p*q
         q0 = q – 1./3. *p**2
         dis = (r0/2.)**2 + (q0/3.)**3
         if (dis.gt.0.0) then
            reg1 = sqrt(dis)
            reg2 = reg1 – r0/2.0
            reg3 = reg1 + r0/2.0
            if (reg2 .gt. 0.0) then
                reg2 = reg2**(1./3.)
            else
                reg2 = -(-reg2)**(1./3.)
            endif
            if (reg3 .gt. 0.0) then
                reg3 = reg3**(1./3.)
            else
                reg3 = -(-reg3)**(1./3.)
            endif
            l_ci(I,j,k) = sqrt(3.)/2.0*(reg2 + reg3)
         else
            l_ci(I,j,k) = 0.0
         endif
1    continue

     return
     end
```

APPENDIX C

NAVIER-STOKES SOLUTION

This code solves the incompressible, constant viscosity Navier-Stokes equation in a channel flow geometry of height h and imposed pressure gradient dP/dx=1. The variables in the code are all made non-dimensional by the wall friction velocity and the viscous length scale, c.f. equations (1.1 a) and (1.1 b) in the text. The solution is performed by Fourier spectral decomposition in the x- and z-directions, and Chebychev polynomials in the y-direction. The grid is 128 x 129 x 128.

Input variable to the code are:

u.ini, v.ini, w.ini (the initial condition given by the LSE code)

Output variables are fluctuating u, v and w velocities and pressure for every "idmpfrq" iterations (the u,v,w and p values are typically written every 500 iterations which is equivalent to 25 time units).idmpfrq and the total number of timesteps are defined in the APPENDIX D code.

The time step is given by dt=1.25e-04. It is set in APPENDIX D.

The code calls the initial condition from the folder ic_data (refer "set directory from argument" in code below).

```
!c--  07/22/06
!c    irstrt is removed.
!c     to preserve second-order temporal accuarcy between succesive runs,
!c    the nonlinear terms are read from the file such as fu.ini,
fcxx.ini, etc.
!c    time history of cij is added.

!c--  07/31/07
!c    write pressure is added
!c    n+1 and n-1 step fields are written to calculate time-derivatives

!c-- 09/19/09
!c   actual pressure is written instead of dt*p
!c   not to write fu.ini, fcxx.ini, etc

!c-- 09/27/09
!c   read n_ini, time for succesive calculation

!c-- 10/09/09
!c   change dPdx linearly in time

!c-- 10/19/09
!c   employing dump_data logical variable


!c=====================================================================
==
      program main
```

```
      use parameters
      use new_derivatives
      use wave_numbers_stuf
      use general_stuf
      use fftw_routines
      use xyzfft
!c-----------------------------------------------------------------------
--
!c    main program  for turbulent channel flow
!c    allowing to split 1 or 2 dimensions over the processors
!c    data storage: us(nyp,kcomy) = us(nyp,nkz,kxh) etc
!c-----------------------------------------------------------------------
--
      implicit none
      include 'mpif.h'

      complex(8), dimension (1:nyp,1:kcomy) :: us, vs, ws
      complex(8), dimension (1:nyp,1:kcomy) :: u, v, w
      complex(8), dimension (1:nyp,1:kcomy) :: pressure
      complex(8), dimension (1:nyp,1:kcomy) :: temp1,temp2,temp3
      complex(8), dimension (1:nyp,1:kcomy) :: temp

!c--- non-linear term at (n) and (n-1) steps
      complex(8), dimension (1:nyp,1:kcomy) :: fnm, gnm, hnm
      complex(8), dimension (1:nyp,1:kcomy) :: fn, gn, hn
      common/block1/ fnm, gnm, hnm
      common/block5/ fn, gn, hn

!c--- boundary conditions
      complex(8), dimension (1:kcomy) :: bctop, bcbot, pbctop, pbcbot

!c--- influence matrix for helmholtz eq
      real(8), dimension (0:ny,1:kcomy) :: a, ag, ac
      real(8), dimension (1:kcomy) ::  wn, wng, wnc
      real(8), dimension (1:ny) ::  wd, wl, wr

!c--- the flow variables in physical space
      real(8), dimension (1:nx,1:kcomx) :: srxxp,srxyp,srxzp
      real(8), dimension (1:nx,1:kcomx) :: sryyp,sryzp,srzzp
      real(8), dimension (1:nx,1:kcomx) :: dxtp, dytp, dztp
      real(8), dimension (1:nx,1:kcomx) :: rxxp, rxyp, rxzp
      real(8), dimension (1:nx,1:kcomx) :: ryyp, ryzp, rzzp
      real(8), dimension (1:nx,1:kcomx) :: omxp, omyp, omzp
      real(8), dimension (1:nx,1:kcomx) :: up, vp, wp

      real(8) :: cfl_max, div_max, re_m, time

!c--- for cpu time measuring
      real(4) :: cpu_start, cpu_end, cpu_proc, cpu_sum, cpu_max

!c--- mpi related constant
      integer ierr, nprocmpi
      integer mynum
      common/cbpar2/ mynum
```

```
!c--- indicies and coefficients
      integer :: i, iy, izx, it, in, n_ini
      integer :: ibp, ib, error
      real(8) :: g, sg, sa, con_1, con_2

!c--- input and output file names
      character(len=70), dimension (1:99) :: namein, nameout

!c--- fene-p model
      complex(8), dimension (1:nyp,1:kcomy) :: cxx,cxy,cxz,cyy,cyz,czz
      complex(8), dimension (1:nyp,1:kcomy) :: c_fnxx, c_fnxy, c_fnxz
      complex(8), dimension (1:nyp,1:kcomy) :: c_fnyy, c_fnyz, c_fnzz
      complex(8), dimension (1:nyp,1:kcomy) :: c_fnmxx,c_fnmxy,c_fnmxz
      complex(8), dimension (1:nyp,1:kcomy) :: c_fnmyy,c_fnmyz,c_fnmzz

!c--- pressure gradient change
      integer :: time_region
      real(8) :: re_tau_time
      real(8) :: dpdx_time

      logical :: dump_data

!c--- directory input (JRB)
      character*30 :: dirarg
      integer :: iargc


!c-----------------------------------------------------------------------
--
!c    mpi initializations
!c-----------------------------------------------------------------------
--
      if ( nproc > 1 ) then
           call mpi_init( ierr )
           if ( ierr /= 0 ) stop "init 1"
           call mpi_comm_rank( mpi_comm_world, mynum, ierr )
           if ( ierr /= 0 ) stop "init 2"
           call mpi_comm_size( mpi_comm_world, nprocmpi, ierr )
           if ( ierr /= 0 ) stop "init 3"
           if ( nprocmpi /= nproc ) stop 'error nproc'
           if ( mod(nxh,nproc) /= 0 ) stop " invalid nproc: see nxh (1)
"
           if ( mod(nz,nproc)  /= 0 ) stop " invalid nproc: see nz "
      else
           mynum = 0
      endif

!c----------------------------
!c     set directory from argument
!c--------------------------------
      if (iargc().ne.1) stop "must set argument: <program> <######>"
      call getarg(1,dirarg)
      folder_in="ic_data"//trim(dirarg)//"/"
      folder_out="/scratch/pkvraman/output"//trim(dirarg)//"/"
```

```
      write(*,*) "folder_in  > ", trim(folder_in)
      write(*,*) "folder_out > ", trim(folder_out)

!c-----------------------------------------------------------------------
--
!c    setup
!c-----------------------------------------------------------------------
--
      call setstuf
      if( .not.solve_fenep_model .and. beta /= 1.d0 ) stop "beta"

!c-----------------------------------------------------------------------
--
!c    define the input/output arrays
!c-----------------------------------------------------------------------
--
      namein(1) = "u"
      namein(2) = "v"
      namein(3) = "w"
      namein(4) = "cxx"
      namein(5) = "cxy"
      namein(6) = "cxz"
      namein(7) = "cyy"
      namein(8) = "cyz"
      namein(9) = "czz"
      namein(10) = "p"

      namein(11) = "fu"
      namein(12) = "fv"
      namein(13) = "fw"
      namein(14) = "fcxx"
      namein(15) = "fcxy"
      namein(16) = "fcxz"
      namein(17) = "fcyy"
      namein(18) = "fcyz"
      namein(19) = "fczz"

      nameout = namein

      do i = 1, 19
         namein(i)  = trim(folder_in )//trim(namein(i) )//".ini"
         nameout(i) = trim(folder_out)//trim(nameout(i))//"."
      enddo

!c-----------------------------------------------------------------------
--
!c    initialisations for fft routines
!c-----------------------------------------------------------------------
--
      call xyzfft_ini
      call ccosexp_trig

!c-----------------------------------------------------------------------
--
!c    set up the boundary conditions at y = [-1, 1] for channel flow
```

```
!c    always check for consistency the pressure bcs for the zero mode
!c    (dp/dy(1)-dp/dy(-1))*dyde = v(1) - v(-1)
!c-----------------------------------------------------------------------
--
      bctop  = dcmplx(0.0d0, 0.0d0)
      bcbot  = dcmplx(0.0d0, 0.0d0)
      pbctop = dcmplx(0.0d0, 0.0d0)
      pbcbot = dcmplx(0.0d0, 0.0d0)

      n_ini = 0    ! if n_ini is not 0, the initial files for nonlinear
terms at (n-1) step are required.
      time = 0.0d0

!c--- for interactive job
!c    read (*,*) n_ini
!c    read (*,*) time
      n_ini=0
      time=0.0

      write(*,*) mynum, n_ini, time
!c---

!c-----------------------------------------------------------------------
--
!c    read initial data
!c-----------------------------------------------------------------------
--

                call var_scatter( u, namein(1) )
                call var_scatter( v, namein(2) )
                call var_scatter( w, namein(3) )
!c            if ( n_ini .ne. 0 ) then
!c                 call var_scatter( fnm, namein(11) )   ! for
continuous calculation  07/21/06
!c                 call var_scatter( gnm, namein(12) )
!c                 call var_scatter( hnm, namein(13) )
!c            endif

            if ( solve_fenep_model ) then
                call var_scatter( cxx, namein(4) )
                call var_scatter( cxy, namein(5) )
                call var_scatter( cxz, namein(6) )
                call var_scatter( cyy, namein(7) )
                call var_scatter( cyz, namein(8) )
                call var_scatter( czz, namein(9) )
!c            if ( n_ini .ne. 0 ) then
!c                 call var_scatter( c_fnmxx, namein(14) )
!c                 call var_scatter( c_fnmxy, namein(15) )
!c                 call var_scatter( c_fnmxz, namein(16) )
!c                 call var_scatter( c_fnmyy, namein(17) )
!c                 call var_scatter( c_fnmyz, namein(18) )
!c                 call var_scatter( c_fnmzz, namein(19) )
!c            endif
            endif
```

```
!c-----------------------------------------------------------------
--
!c    initialize the influence matrix in initial.
!c-----------------------------------------------------------------
--
      call initial( pressure, temp, &
                    bctop, bcbot, a, ag, ac, wn, wng, wnc, wd, wl, wr,
pbctop, pbcbot)

!c--- write simulation parameters

      if ( nproc >  1 ) call mpi_barrier( mpi_comm_world, ierr )
      if ( mynum == 0 ) then
           write(*,*)
           write(*,*) '-----------------------------------', &
                      ' parameters ',                      &
                      '-----------------------------------'
           write(*,*) 're_tau = ', re_tau
           if ( scale_by_pi ) then
                write(*,*) 'len_x = ', xl * acos(-1.0)
                write(*,*) 'len_z = ', zl * acos(-1.0)
           else
                write(*,*) 'len_x = ', xl
                write(*,*) 'len_z = ', zl
           endif
           write(*,*) 'nx = ', nx
           write(*,*) 'ny = ', ny
           write(*,*) 'nz = ', nz
           write(*,*) 'dt = ', dt
           write(*,*) 'nproc = ', nproc
           if ( solve_fenep_model ) then
                write(*,*) 'we_tau = ', we_tau
                write(*,*) 'beta   = ', beta
                write(*,*) 'l_max  = ', lmax
                write(*,*) 'diffusivity = ', diffusivity
           endif
           write(*,*)
           write(*,*) '-----------------------------------', &
                      ' program starts ',                    &
                      '-----------------------------------'
           write(*,*)
      endif


!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++
!c    main time stepping loop
!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++

      call cpu_time( cpu_start )

      do it = n_ini + 1, n_ini + nsteps
```

```
!c-----------------------------------------------------------------
---
!c    calculate the vorticity, strain-rate tensor and velocity in
physical domain.
!c-----------------------------------------------------------------
---
         call vort1( u, v, w, omxp, omyp, omzp )
         call gadot( u, v, w,
srxxp ,srxyp ,srxzp ,sryyp ,sryzp ,srzzp )

         call xyzfftsp( u, up )
         call xyzfftsp( v, vp )
         call xyzfftsp( w, wp )

         call divergence( div_max, srxxp, sryyp, srzzp )
         call cfl_number( cfl_max, up, vp, wp )

         if ( mynum == 0 ) call mean_reynolds_number( re_m, u, time )
         if ( mynum == 0 ) call time_history( up, vp, wp, time )

         if ( mynum == 0 ) then
              write(*,100) it-1, time, re_m, div_max, cfl_max
100           format(' step =',i7,2x,':  t =',e15.9,2x,' re_m
=',e15.9,2x, &
                      ' div =',e15.9,2x,' cfl =',e15.9)
         endif

         time = time + dt

!c-----------------------------------------------------------------
---
!c    adams-bashforth  for it > 1
!c    bacward euler    for it = 1 and read the array of filled zero
!c-----------------------------------------------------------------
---
!c         if ( it == 1 ) then
         if ( it == n_ini + 1 ) then
              con_1 = dt
              con_2 = 0.d0

              fnm=0.d0; gnm=0.d0; hnm=0.d0
              c_fnmxx=0.d0; c_fnmxy=0.d0; c_fnmxz=0.d0
              c_fnmyy=0.d0; c_fnmyz=0.d0; c_fnmzz=0.d0
         else
              con_1 = + 1.5d0*dt
              con_2 = - 0.5d0*dt
         endif

!c--- store spectral coefficient u^(n) to us
         forall( izx=1:kcomy, iy=1:nyp )
                 us(iy,izx) = u(iy,izx)
                 vs(iy,izx) = v(iy,izx)
                 ws(iy,izx) = w(iy,izx)
         endforall
```

```
!c-----------------------------------------------------------------
---
!c    polymer stress
!c-----------------------------------------------------------------
---
         if ( solve_fenep_model ) then

              call get_polymer_stress ( cxx, cyy, czz,             & !
in: cij at n, out: cij at n+1
                                        cxy, cxz, cyz,             &
                                        c_fnxx, c_fnyy, c_fnzz,    & !
out: polymer stress at n+1
                                        c_fnxy, c_fnxz, c_fnyz,    &
                                        c_fnmxx, c_fnmyy, c_fnmzz, & !
fij at n-1 in step 1 of fenep
                                        c_fnmxy, c_fnmxz, c_fnmyz, &
                                        omxp, omyp, omzp,          &
                                        srxxp, sryyp, srzzp,       &
                                        srxyp, srxzp, sryzp,       &
                                        up, vp, wp,                &
                                        con_1, con_2,              &
                                        ac, wnc, wd, wl, wr,       &
                                        time )

!c--- update the polymer stress contrinution

              sa = (1.d0-beta)*(dt/2.d0)/re_tau
              do i = 1, kcomy

                 u(:,i) = u(:,i) + sa*(  x_der_1(c_fnxx(:,i),i)  &
                                       + y_der_1(c_fnxy(:,i))    &
                                       + z_der_1(c_fnxz(:,i),i))

                 v(:,i) = v(:,i) + sa*(  x_der_1(c_fnxy(:,i),i)  &
                                       + y_der_1(c_fnyy(:,i))    &
                                       + z_der_1(c_fnyz(:,i),i))

                 w(:,i) = w(:,i) + sa*(  x_der_1(c_fnxz(:,i),i)  &
                                       + y_der_1(c_fnyz(:,i))    &
                                       + z_der_1(c_fnzz(:,i),i))
              enddo

         endif


!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++
!c    stage 1
!c    compute the nonlinear terms for the momentum equations.
!c    this part calculates the nonlinear term in
!c    the skew-symmetric form.
!c    i.e, u.grad u = 1/2 ( u.grad u + div (uu) )
!c    evaluate all terms at old time, including viscous term
!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++
```

```
         do i = 1, kcomx

!c--- -( u.grad (u))/2 part

            dxtp(:,i) = -(   up(:,i)* srxxp(:,i)             &
                           + vp(:,i)*(srxyp(:,i)-omzp(:,i))  &
                           + wp(:,i)*(srxzp(:,i)+omyp(:,i))  &
                         )/4.0d0
            dytp(:,i) = -(   vp(:,i)* sryyp(:,i)             &
                           + up(:,i)*(srxyp(:,i)+omzp(:,i))  &
                           + wp(:,i)*(sryzp(:,i)-omxp(:,i))  &
                         )/4.0d0

            dztp(:,i) = -(   wp(:,i)* srzzp(:,i)             &
                           + up(:,i)*(srxzp(:,i)-omyp(:,i))  &
                           + vp(:,i)*(sryzp(:,i)+omxp(:,i))  &
                         )/4.0d0

!c--- -(div (uu))/2 part : gradient will be applied later

            rxxp(:,i) = -up(:,i)*up(:,i)/2.d0
            rxyp(:,i) = -up(:,i)*vp(:,i)/2.d0
            rxzp(:,i) = -up(:,i)*wp(:,i)/2.d0
            ryyp(:,i) = -vp(:,i)*vp(:,i)/2.d0
            ryzp(:,i) = -vp(:,i)*wp(:,i)/2.d0
            rzzp(:,i) = -wp(:,i)*wp(:,i)/2.d0

         enddo

         call xyzfftps( dxtp, fn )
         call xyzfftps( dytp, gn )
         call xyzfftps( dztp, hn )

         call xyzfftps( rxxp, c_fnxx )
         call xyzfftps( rxyp, c_fnxy )
         call xyzfftps( rxzp, c_fnxz )
         call xyzfftps( ryyp, c_fnyy )
         call xyzfftps( ryzp, c_fnyz )
         call xyzfftps( rzzp, c_fnzz )

         g = dt/(2*re_tau) * beta ! for newtonian fluid beta = 1.d0

         do i = 1, kcomy
            fn(:,i) = fn(:,i) + x_der_1(c_fnxx(:,i),i) +
y_der_1(c_fnxy(:,i)) + z_der_1(c_fnxz(:,i),i)
            gn(:,i) = gn(:,i) + x_der_1(c_fnxy(:,i),i) +
y_der_1(c_fnyy(:,i)) + z_der_1(c_fnyz(:,i),i)
            hn(:,i) = hn(:,i) + x_der_1(c_fnxz(:,i),i) +
y_der_1(c_fnyz(:,i)) + z_der_1(c_fnzz(:,i),i)

!c--- adams - bashforth integration
            u(:,i) = u(:,i) + con_1*fn(:,i) + con_2*fnm(:,i)
            v(:,i) = v(:,i) + con_1*gn(:,i) + con_2*gnm(:,i)
            w(:,i) = w(:,i) + con_1*hn(:,i) + con_2*hnm(:,i)
```

```
!c--- save the convection term  for the next time-step in adams-
bashford
            fnm(:,i) = fn(:,i)
            gnm(:,i) = gn(:,i)
            hnm(:,i) = hn(:,i)

!c--- add viscous corrections to u(n), v(n), w(n)
            u(:,i)=u(:,i) +
g*(x_der_2(us(:,i),i)+y_der_1(y_der_1(us(:,i)))+z_der_2(us(:,i),i))
            v(:,i)=v(:,i) +
g*(x_der_2(vs(:,i),i)+y_der_1(y_der_1(vs(:,i)))+z_der_2(vs(:,i),i))
            w(:,i)=w(:,i) +
g*(x_der_2(ws(:,i),i)+y_der_1(y_der_1(ws(:,i)))+z_der_2(ws(:,i),i))

         enddo


!c++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++
!c    stage 2
!c    the pressure step  (n + 1/3   to   n + 2/3)
!c++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++

         call get_pressure ( pressure, u, v, w,                  &
                             pbctop, pbcbot, a, wn, wd, wl, wr, &
                             bctop, bcbot, ag, wng  )

!c--- update velocity at (n+2/3)
         forall( i = 1:kcomy )
                 u(:,i) = u(:,i) - x_der_1( pressure(:,i),i )
                 v(:,i) = v(:,i) - y_der_1( pressure(:,i)   )
                 w(:,i) = w(:,i) - z_der_1( pressure(:,i),i )
         endforall

!c--- apply constant pressuregradient in x-direction
!c         if ( mynum==0 ) u(1,1) = u(1,1) + dt


!c--- pressure gradient change
         if ( mynum==0 ) then

             time_region = 1
             if (time.ge.time_s .and. time.lt.time_f) time_region = 2
             if (time.ge.time_f ) time_region = 3

             select case(time_region)
               case(1)
                   dpdx_time = 1.0
               case(2)
                   dpdx_time = ((re_tau_final/re_tau)**2 -
1.0)/(time_f-time_s)*(time-time_s)+1.0
               case(3)
                   dpdx_time = (re_tau_final/re_tau)**2
```

```
            end select

            u(1,1) = u(1,1) + dt * dpdx_time

         endif


!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++
!c    stage 3
!c    calculate velocities at (n + 1)
!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++

!c--- u^(n+1)
         sg = -2.0d0*re_tau/dt/beta
         forall( i = 1:kcomy )
                 temp(:,i)         = sg * u(:,i)
                 temp(nyp-3:nyp,i) = (0.d0,0.d0)
         endforall

         in = 0;  g  = 2.0d0*re_tau/dt/beta;  ib = 0
         call solve( temp, u,        &             ! input/output
                     g, dyde, in,    &             ! input
                     bctop, bcbot,ib,wavz, wavx, ag, wng, wd, wl,
wr )  ! input/output
!c--- v^(n+1)
         sg = -2.0d0*re_tau/dt/beta
         forall( i = 1:kcomy )
                 temp(:,i)         = sg * v(:,i)
                 temp(nyp-3:nyp,i) = (0.d0,0.d0)
         endforall

         in = 0;  g  = 2.0d0*re_tau/dt/beta;  ib = 0
         call solve( temp, v,        &             ! input/output
                     g, dyde, in,    &             ! input
                     bctop, bcbot,ib,wavz, wavx, ag, wng, wd, wl,
wr )  ! input/output
!c--- w^(n+1)
         sg = -2.0d0*re_tau/dt/beta
         forall( i = 1:kcomy )
                 temp(:,i)         = sg * w(:,i)
                 temp(nyp-3:nyp,i) = (0.d0,0.d0)
         endforall

         in = 0;  g  = 2.0d0*re_tau/dt/beta;  ib = 0
         call solve( temp, w,        &             ! input/output
                     g, dyde, in,    &             ! input
                     bctop, bcbot,ib,wavz, wavx, ag, wng, wd, wl,
wr )  ! input/output

!c---------------------------------------------------------------------
--
!c    output of data required for restart
```

```
!c-----------------------------------------------------------------------
--

         dump_data = .false.
         dump_data = ((mod(it,idmpfrq) == 0) .or. (it == nsteps +
n_ini))

         if (time.ge.time_s .and. time.le.time_f) then

            if ( mod( int((time-time_s)/dt+0.5)*60, int((time_f-
time_s)/dt+0.5) )==0  &
               ) dump_data  = .true.

         endif

         if ( dump_data  &

!         if ( mod(it,idmpfrq) == 0 .or. it == nsteps + n_ini   &
!c         .or. mod(it-1,idmpfrq) == 0 .or. mod(it+1,idmpfrq) == 0   &
             ) then
                  call dooutputs( u,   nameout(1), it )
                  call dooutputs( v,   nameout(2), it )
                  call dooutputs( w,   nameout(3), it )
                  call dooutputs( pressure/dt, nameout(10), it )

!                  call dooutputs( fnm,   nameout(11), it )
!                  call dooutputs( gnm,   nameout(12), it )
!                  call dooutputs( hnm,   nameout(13), it )
             if ( solve_fenep_model ) then
                  call dooutputs( cxx, nameout(4), it )
                  call dooutputs( cxy, nameout(5), it )
                  call dooutputs( cxz, nameout(6), it )
                  call dooutputs( cyy, nameout(7), it )
                  call dooutputs( cyz, nameout(8), it )
                  call dooutputs( czz, nameout(9), it )

!                  call dooutputs( c_fnmxx, nameout(14), it )
!                  call dooutputs( c_fnmxy, nameout(15), it )
!                  call dooutputs( c_fnmxz, nameout(16), it )
!                  call dooutputs( c_fnmyy, nameout(17), it )
!                  call dooutputs( c_fnmyz, nameout(18), it )
!                  call dooutputs( c_fnmzz, nameout(19), it )
             endif
         endif

      enddo  ! time-steps

!c--- cpu time for all processors
      call cpu_time( cpu_end )
      cpu_proc = cpu_end - cpu_start

      if ( nproc > 1 ) then
           call mpi_reduce( cpu_proc, cpu_sum, 1, mpi_real, &
                            mpi_sum, 0, mpi_comm_world, ierr)
           call mpi_reduce( cpu_proc, cpu_max, 1, mpi_real, &
```

```
                          mpi_max, 0, mpi_comm_world, ierr)
      else
           cpu_sum = cpu_proc
           cpu_max = cpu_proc
      endif

      if ( mynum == 0 ) then
           write(*,*)
           write(*,*) ' total cpu time over all processors =
',int(cpu_sum/60.+1),' mins'
           write(*,*) ' wall clock time                    =
',int(cpu_max/60.+1),' mins'
           write(*,*)
      endif


!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++
!c    end main loop
!c+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++

      if ( nproc > 1 ) then
           call mpi_barrier( mpi_comm_world, ierr )
           call mpi_finalize( ierr )
      endif

      end program main

!c=====================================================================
=
      subroutine setstuf
      use parameters
      use wave_numbers_stuf
      use general_stuf

      implicit none

      integer mynum
      common/cbpar2/ mynum

      integer j, jstart, jz, k, keff, nxi, nyi, nzi
      real(8) wavzall(nz)
      real(8) alpha, bhta, rj, rn

!c---------------------------------------------------------------------
--
!c    calculate the resolvable wave nos. in x:
!c    assumes length xl has been non-dimensionalized with the length
yhl.
!c---------------------------------------------------------------------
--
      pi = 4.d0 * datan(1.d0)

      if ( scale_by_pi ) then
```

```
          alpha = 2.0d0/xl
          bhta  = 2.0d0/zl
      else
          alpha = 2.0d0*pi/xl
          bhta  = 2.0d0*pi/zl
      endif
!c-----------------------------------------------------------------------
--
!c    each processor, in the spectral domain consists of data in
!c    the form : complex a(nyp,kcomy) = a(nyp,nkz,kxh)
!c    so for the x-derivative, between 1 and nxh/nproc wave numbers
!c    are used per processor for nproc larger and smaller than
!c    nxh respectively
!c    for the z derivatives, between (nz*nxh)/nproc and nz wave numbers
!c    are used per processor for nproc larger and smaller than
!c    nxh respectively
!c-----------------------------------------------------------------------
--
      do k = 1, kxh
         keff     = (mynum*nxh)/nproc + k - 1
         wavx(k)  = dfloat(keff)*alpha
         cwavx(k) = dcmplx(0.0d0, 1.0d0)*wavx(k)
         wavx2(k) = -wavx(k)*wavx(k)
      enddo
!c-----------------------------------------------------------------------
--
!c    first calculate all possible wavz
!c    then select proper values for current processor mynum
!c    distinguish nproc > nxh and nproc <= nxh
!c-----------------------------------------------------------------------
--
      do j = 1, max0(1,nz/2)
         wavzall(j) = dfloat(j-1)*bhta
      enddo
      do j = nz/2 + 1, nz
         wavzall(j) = dfloat(j-2*(nz/2)-1)*bhta
      enddo

      if ( kxh == 1 ) then
          jz = mod(mynum,kproc_yz)
          jstart = jz * kcomy
      else
          jstart = 0
      endif

      do j = 1, nkz
         wavz(j)  = wavzall(j+jstart)
         cwavz(j) = dcmplx(0.0d0, 1.0d0)*wavz(j)
         wavz2(j) = - wavz(j)*wavz(j)
      enddo

      end subroutine setstuf

!c=====================================================================
==
```

```
      subroutine diverg( u, v, w, div )
!c-----------------------------------------------------------------------
--
!c    this subroutine calculates fourier/chebyshev coeff of divergence
!c    input and output are fourier/chebyshev coefficients.
!c-----------------------------------------------------------------------
--
      use parameters, only : nyp,kcomy
      use new_derivatives
      implicit none

      complex(8),intent(in),  dimension (nyp,kcomy) :: u, v, w
      complex(8),intent(out), dimension (nyp,kcomy) :: div

      integer :: i

      forall( i = 1:kcomy )

div(:,i)=x_der_1(u(:,i),i)+y_der_1(v(:,i))+z_der_1(w(:,i),i)
      endforall

      end subroutine diverg

!c=====================================================================
==
      subroutine vort1( ux, uy, uz, omxp, omyp, omzp )
!c-----------------------------------------------------------------------
--
!c    calculate vorticity components and transformed to physical values
!c-----------------------------------------------------------------------
--
      use parameters
      use new_derivatives
      use xyzfft
      implicit none

      complex(8),intent(in), dimension (nyp,kcomy):: ux, uy, uz
      real(8)   ,intent(out),dimension (nx,kcomx) :: omxp,omyp,omzp

      complex(8),dimension (nyp,kcomy) :: temp
      integer :: i

      forall( i = 1:kcomy )
              temp(:,i) = x_der_1(uy(:,i),i) - y_der_1(ux(:,i))
      endforall
      call xyzfftsp(temp, omzp)

      forall( i = 1:kcomy )
              temp(:,i) = y_der_1(uz(:,i)) - z_der_1(uy(:,i),i)
      endforall
      call xyzfftsp(temp, omxp)

      forall( i = 1:kcomy )
              temp(:,i) = z_der_1(ux(:,i),i) - x_der_1(uz(:,i),i)
      endforall
```

```
      call xyzfftsp(temp, omyp)

      end subroutine vort1

!c=====================================================================
==
      subroutine gadot(ux,uy,uz,srxxp,srxyp,srxzp,sryyp,sryzp,srzzp)
!c---------------------------------------------------------------------
--
!c    calculate strain-rate tensors and transformed to physical values
!c    (e.g.) srxyp =  dux/dy + duy/dx
!c---------------------------------------------------------------------
--
      use parameters
      use new_derivatives
      use xyzfft
      implicit none

      complex(8),intent(in),dimension(nyp,kcomy) :: ux, uy, uz
      real(8),  intent(out),dimension(nx,kcomx)  :: srxxp, srxyp, srxzp
&
                                                   ,sryyp, sryzp, srzzp

      complex(8),dimension(nyp,kcomy)     :: temp
      integer :: i

      forall( i = 1:kcomy )
              temp(:,i) = 2.d0*x_der_1(ux(:,i),i)
      endforall
      call xyzfftsp(temp,srxxp)

      forall( i = 1:kcomy )
              temp(:,i) = 2.d0*y_der_1(uy(:,i))
      endforall
      call xyzfftsp(temp,sryyp)

      forall( i = 1:kcomy )
              temp(:,i) = 2.d0*z_der_1(uz(:,i),i)
      endforall
      call xyzfftsp(temp,srzzp)

      forall( i = 1:kcomy )
              temp(:,i) = x_der_1(uy(:,i),i) + y_der_1(ux(:,i))
      endforall
      call xyzfftsp(temp,srxyp)

      forall( i = 1:kcomy )
              temp(:,i) = x_der_1(uz(:,i),i) + z_der_1(ux(:,i),i)
      endforall
      call xyzfftsp(temp,srxzp)

      forall( i = 1:kcomy )
              temp(:,i) = z_der_1(uy(:,i),i) + y_der_1(uz(:,i))
      endforall
      call xyzfftsp(temp,sryzp)
```

```
      end subroutine gadot

!c=====================================================================
==
      subroutine var_scatter( varo, nameins )
      use parameters
      implicit none
      include 'mpif.h'

      complex(8) varo(nyp,kcomy)
      character(len=*), intent(in) :: nameins

      integer mynum
      common/cbpar2/ mynum

      complex(8), dimension (nyp,nz,nxh) :: vari
      integer i, icomy, ierr, j, k

      if ( mynum == 0 ) then
           write(*,*) ' reading initial data : ', nameins

open(21,file=nameins,status="old",action="read",form='unformatted')
           read(21) (((vari(j,k,i),j=1,nyp),k=1,nz),i=1,nxh)
           close(21)
      endif

          if ( nproc > 1 ) then
               call mpi_barrier( mpi_comm_world, ierr )
               call mpi_scatter( vari, kdata, mpi_double_complex, varo,
kdata, mpi_double_complex, &
                                 0, mpi_comm_world, ierr )
      elseif ( nproc == 1 ) then
               do i = 1, nxh
               do k = 1, nz
               do j = 1, nyp
                  icomy = k + (i-1)*nz
                  varo(j,icomy) = vari(j,k,i)
               enddo
               enddo
               enddo
      endif

      end subroutine var_scatter

!c=====================================================================
      subroutine dooutputs( qs, nameouts, it )
!c---------------------------------------------------------------------
!c    gather the data of the processors to processor 0 for output
!c    and write in a file
!c---------------------------------------------------------------------
      use parameters
      use general_stuf
      use xyzfft
      implicit none
```

```
      include 'mpif.h'

      complex(8),intent(in),dimension(nyp,kcomy) :: qs
      character(len=70),intent(in) :: nameouts
      character(len=70)            :: filename

      integer mynum
      common/cbpar2/ mynum
      complex(8),dimension (nyp,nz,nxh) :: qsall
      integer :: i, icomy, ierr, j, k, it

          if ( nproc > 1 ) then
               call mpi_barrier( mpi_comm_world, ierr )
               call mpi_gather( qs, kdata, mpi_double_complex, qsall,
kdata, mpi_double_complex, 0, &
                                mpi_comm_world, ierr )
      elseif ( nproc == 1 ) then
               do i = 1, nxh
               do k = 1, nz
               do j = 1, nyp
                  icomy = k + (i-1)*nz
                  qsall(j,k,i) = qs(j,icomy)
               enddo
               enddo
               enddo
      endif

      if ( mynum == 0 ) then

           filename = nameouts
           i=index(filename,'.')
!           write(unit=filename(i+1:),fmt='(bn,i5.5)') it
!           write(unit=filename(i+1:),fmt='(bn,i6.6)') it
           write(unit=filename(i+1:),fmt='(bn,i7.7)') it
           write(*,*) 'writing file: ', filename


open(31,file=filename,status="unknown",action="write",form='unformatted
')
           write(31) (((qsall(j,k,i),j=1,nyp),k=1,nz),i=1,nxh)
           close(31)
      endif

      if ( nproc > 1 ) call mpi_barrier( mpi_comm_world, ierr )

      end subroutine dooutputs

!c=====================================================================
!      subroutine mean_reynolds( spec, name, time )
      subroutine mean_reynolds_number( re_m, spec, time )
      use parameters
      use general_stuf
      implicit none

      complex(8), intent(in), dimension (nyp,kcomy) :: spec
```

```
!      character(len=*), intent(in) :: name
      real(8)  time

      real(8)  :: re_m  ! = u_m*(2h)/nu
      integer :: iy

         re_m = 0.d0
      do iy = 0, nyp-1, 2
         re_m = re_m + real(spec(iy+1,1),8)/dble(1-iy*iy)*2.0d0
      enddo
         re_m = re_m * re_tau

      open (10, file=trim(folder_out)//'time_hist_re_m.dat',
position="append", action="write")
      write(10,"(e15.9,x,e15.9)") time, re_m
      close(10,status="keep")

      end subroutine mean_reynolds_number

!c=====================================================================
      subroutine cfl_number( cfl_max, up, vp, wp )
      use parameters
      use general_stuf
      implicit none
      include 'mpif.h'

      real(8), dimension (1:nx,1:kcomx) :: up, vp, wp

      real(8) :: cfl_max, cfl_max_proc, cfl_local
      real(8) :: delta_x, delta_z, delta_y

      integer i, j, k, icomx, ierr

      pi = 4.d0 * datan(1.d0)

      if ( scale_by_pi ) then
           delta_x = xl * pi / dble(nx)
           delta_z = zl * pi / dble(nz)
      else
           delta_x = xl / dble(nx)
           delta_z = zl / dble(nz)
      endif

      cfl_max_proc = 0.d0

      do icomx = 1, kcomx
         do i = 1, nx

            j = mod( icomx - 1, nyp) + 1

            delta_y =  cos(dble(j-1)*pi/dble(ny)) &
                     - cos(dble(j  )*pi/dble(ny))

            cfl_local =  abs(up(i,icomx))/delta_x  &
                       + abs(vp(i,icomx))/delta_y  &
```

```
                        + abs(wp(i,icomx))/delta_z
            if ( cfl_local .gt. cfl_max_proc )  cfl_max_proc =
cfl_local
         enddo
      enddo

      cfl_max_proc = cfl_max_proc * dt

      if ( nproc > 1 ) then
           call mpi_reduce( cfl_max_proc, cfl_max, 1,
mpi_double_precision, &
                            mpi_max, 0, mpi_comm_world, ierr)
      else
           cfl_max = cfl_max_proc
      endif

      end subroutine cfl_number

!c=====================================================================
      subroutine time_history( up, vp, wp, time )
      use parameters
      use general_stuf
      implicit none

      real(8), dimension (1:nx,1:kcomx) :: up, vp, wp
      real(8) time
      integer :: i, j, k, icomx(4)

!c--- monitoring points
      i = 1
      k = 1   ! should be less than kz

      j = 2
      icomx(1) = (k - 1)*nyp + j

      j = 10
      icomx(2) = (k - 1)*nyp + j

      j = 30
      icomx(3) = (k - 1)*nyp + j

      j = 65
      icomx(4) = (k - 1)*nyp + j

      open (10, file=trim(folder_out)//'time_hist_u.dat',
position="append", action="write")
      write(10, 100) time, (up(i,icomx(k)),k=1,4)
      close(10, status="keep")

      open (10, file=trim(folder_out)//'time_hist_v.dat',
position="append", action="write")
      write(10, 100) time, (vp(i,icomx(k)),k=1,4)
      close(10, status="keep")
```

```
      open (10, file=trim(folder_out)//'time_hist_w.dat',
position="append", action="write")
      write(10, 100) time, (wp(i,icomx(k)),k=1,4)
      close(10, status="keep")

100   format(5(e15.9,x))

      end subroutine time_history

!c=====================================================================
      subroutine divergence( div_max, srxxp, sryyp, srzzp )

      use parameters
      use general_stuf
      implicit none
      include 'mpif.h'

      real(8), dimension (1:nx,1:kcomx) :: srxxp,sryyp,srzzp
      real(8) :: div_max, div_max_proc, div_local
      integer :: i, icomx, ierr

      div_max_proc = 0.d0

      do icomx = 1, kcomx
         do i = 1, nx
            div_local = srxxp(i,icomx) + sryyp(i,icomx) +
srzzp(i,icomx)
            if ( div_local .gt. div_max_proc )  div_max_proc =
div_local
         enddo
      enddo

      div_max_proc = 0.5 * div_max_proc

      if ( nproc > 1 ) then
           call mpi_reduce( div_max_proc, div_max, 1,
mpi_double_precision, &
                            mpi_max, 0, mpi_comm_world, ierr)
      else
           div_max = div_max_proc
      endif

      end subroutine divergence
```

APPENDIX D

This code defines all the parameters used in APPENDIX C.

```
!=========================================================================
      module parameters
!=========================================================================

!-------------------------------------------------------------------------
-
!     parameters for a specific problem
!     nype    array size in y-direction
!     nproc   number of processors, which has to fulfil
!             1) nxh * nz / nproc is integer
!             2) nxh / nproc is integer
!             3) nype / nproc is integer
!             4) nz / nproc is integer
!-------------------------------------------------------------------------
-

      integer, parameter :: nproc = 64    ! number of processors

      integer, parameter :: nx = 128  ! number of points in x-direction
      integer, parameter :: ny = 128 ! number of points in y-direction
      integer, parameter :: nz = 128 ! number of points in z-direction
      integer, parameter :: nxh = nx/2
      integer, parameter :: nyh = ny/2
      integer, parameter :: nyp = ny+1
!      integer, parameter :: nyp_n = ny_n+1
      integer, parameter :: nype = nyp

!-------------------------------------------------------------------------
-
!     derived parameters
!     kcomx      number of yz data per proc for x-array
!     kcomy      number of zx data per proc for y-array
!     kcomz      number of xy data per proc for z-array
!     kdata      number of data per proc
!     kproc_yz   number of procs for the yz communication
!              = number of procs to store z-info for y-array
!     kproc_zx   number of procs for the yz communication = nproc /
kproc_zx
!-------------------------------------------------------------------------
-

      integer, parameter :: kcomx    = (nz*nype)/nproc
      integer, parameter :: kcomy    = (nz*nxh)/nproc
      integer, parameter :: kcomz    = (nype*nxh)/nproc
      integer, parameter :: kdata    = nyp*kcomy
      integer, parameter :: kproc_yz = 1+(nproc-1)/nxh
      integer, parameter :: kproc_zx = nxh

      integer, parameter :: kxh = 1 + (kcomy-1)/nz
      integer, parameter :: kz  = nz / nproc
      integer, parameter :: nkz = kcomy/kxh

      end module parameters
```

```
!=====================================================================
      module general_stuf
!=====================================================================


!       character*8 :: dirarg
!       integer :: iargc
!
character(len=100),parameter::folder_in="ic_data"//trim(dirarg)//"/"
!
character(len=100),parameter::folder_out="/../scratch/output"//trim(dir
arg)//"/"
      character(len=100) :: folder_in
      character(len=100) :: folder_out
      real(8), parameter :: re_tau = 395.d0         ! friction reynolds
number
      integer, parameter :: nsteps =  10000        ! total time steps
      integer, parameter :: idmpfrq =  500        ! frequency to dump
restart files
      real(8), parameter :: dt = 1.25e-04            ! time step
forintegration

      real(8), parameter :: re_tau_final = 395.d0  ! re_tau will be
changed to this value
      real(8), parameter :: time_s = 1d8          ! re_tau will be
changed from this time
      real(8), parameter :: time_f = 1d8 + 10.0     ! re_tau change
will be terminated at this time

      logical, parameter :: scale_by_pi = .true.    ! if true, acutal
xl = xl*pi
      real(8), parameter :: xl   = 2.0d0            ! length in x -
periodic direction
      real(8), parameter :: zl   = 1.0d0            ! length in z -
periodic direction
      real(8), parameter :: yhl  = 2.0d0            ! length in
nonhomogeneous (y) direction

      real(8), parameter :: dyde = 2.0d0/yhl        ! y-scaling factor

      real(8) :: pi

!---------------------------------------------------------------------
--
!     fenep model parameters
!---------------------------------------------------------------------
--

      logical, parameter :: solve_fenep_model = .false.   ! if false,
set beta to be 1.d0
      real(8), parameter :: we_tau      =   25.00d0
      real(8), parameter :: beta        =    1.00d0
      real(8), parameter :: lmax        =    30.00d0 !  b=lmax**2
```

```
      real(8), parameter :: diffusivity =     0.02d0

      real(8), parameter :: we                 = we_tau / re_tau
      real(8), parameter :: diffusivity_factor = 2.d0 / dt /
diffusivity
      real(8), parameter :: lmax_square        = lmax * lmax

      end module general_stuf

!c=====================================================================
===
      module wave_numbers_stuf
!c=====================================================================
===

      use parameters, only : nkz, kxh
      implicit none
      private
      public :: wavz, wavx, cwavz, cwavx, wavz2, wavx2

      real(8),    dimension (nkz) :: wavz
      real(8),    dimension (kxh) :: wavx

      complex(8), dimension (nkz) :: cwavz
      complex(8), dimension (kxh) :: cwavx

      real(8),    dimension (nkz) :: wavz2
      real(8),    dimension (kxh) :: wavx2

      end module wave_numbers_stuf

!c=====================================================================
======
      module new_derivatives
!c=====================================================================
======

      use parameters
      use wave_numbers_stuf

      implicit none
      private

      public :: x_der_1, x_der_2, y_der_1, z_der_1, z_der_2

      contains

!---------------------------------------------------------------------
--------
!              fisrt and second derivatives in x-dir
!              f and df are fourier/chebyshev coefficients.
!---------------------------------------------------------------------
--------

               complex(8) pure function x_der_1( f, icomy ) result (df)
```

```
                implicit none

                integer,    intent(in) :: icomy
                complex(8), intent(in), dimension (1:nyp) :: f
                dimension df(1:nyp)
                integer ix

                ix = ( icomy - 1 ) / nz + 1

                df = cwavx(ix)*f

                end function x_der_1

                complex(8) pure function x_der_2( f, icomy ) result
( ddf )
                implicit none

                integer, intent(in) :: icomy
                complex(8), intent(in), dimension (1:nyp) :: f
                dimension ddf(1:nyp)
                integer ix

                ix = (icomy - 1 ) / nz + 1

                ddf = wavx2(ix)*f

                end function x_der_2


!-----------------------------------------------------------------------
--------
!                df = df/dy   (y = the chebyshev direction)
!                f and df are fourier/chebyshev coefficients.
!-----------------------------------------------------------------------
--------

                complex(8) pure function y_der_1( f ) result ( df )
                implicit none

                complex(8), intent(in),  dimension (1:nyp) :: f
                dimension df(1:nyp)
                integer :: iy

                   df(ny+1) = (0.0d0,0.0d0)
                   df(ny)   = dble(2*ny)*f(nyp)
                do iy = ny-1, 2, -1
                   df(iy) = df(iy+2) + dble(2*iy)*f(iy+1)
                enddo
                   df(1) = 0.5d0*df(3) + f(2)

                end function y_der_1

!-----------------------------------------------------------------------
--------
!               fisrt and second derivatives in z-dir
```

```
!               f and df are fourier/chebyshev coefficients.
!-----------------------------------------------------------------------
--------

                complex(8) pure function z_der_1( f, icomy ) result
( df )
                implicit none

                integer, intent(in) :: icomy
                complex(8), intent(in), dimension (1:nyp) :: f
                dimension df(1:nyp)
                integer ix, iz

                iz = mod(icomy-1, nz) + 1
                ix = ( icomy - 1 ) / nz + 1

                df = cwavz(iz)*f

                end function z_der_1

                complex(8) pure function z_der_2( f, icomy ) result
( ddf )
                implicit none

                integer, intent(in) :: icomy
                complex(8), intent(in), dimension (1:nyp) :: f
                dimension ddf(1:nyp)

                integer ix, iz

                iz = mod(icomy-1, nz) + 1
                ix = ( icomy - 1 ) / nz + 1

                ddf = wavz2(iz)*f

                end function z_der_2

      end module new_derivatives
```

APPENDIX E

VISUALIZATION CODE

This code calculates λ_{ci} (complex eigen value of velocity gradient tensor) for visualizing vortices. It also writes the output velocity files in a readable (tecplot) format.

Grid:128 x 129 x 128;

Re_τ=395;

Language: Fortran 95;

Machine it ran on: Saguaro (ASU high performance computing center);

Number of processors: 1.

Input parameters: u, v, and w components of velocity, components of velocity gradient tensor

Output parameters: λ_{ci} for various t^+.

```
c
c---  write relative value of lambda_ci to its maximum at each flow
field
c
      program channel_post

      include 'param.h'

      common/mesh/y(nyp),dx,dz
      common/domain/sx,sz
      common/para/re
      common/nstep/n_start, n_final, n_skip

      ! directory input (JRB)
      character*30 :: curdir
      integer :: iargc

      if (iargc().ne.1) stop "must set argument: <program> <######>"
      call getarg(1,curdir)
      write(*,*) "current directory > ", trim(curdir)

c---  simulation parameters
      re =  395.
!      re =  180.
!      re = 110.

      pi = acos(-1.0)
!     sx =  4.*pi    !2.*pi !4.*pi    !2.*pi        ! 4.*pi
!     sz =  4.*pi/3  !1.*pi !4.*pi/3  !1./1.*pi     ! 1./1.*pi
```

```
      sx=2.*pi
      sz=1.*pi

c-------------------------------------------

!      read(*,*) n_start
!      read(*,*) n_final
!      read(*,*) n_skip

      n_start = 500 !0
      n_final = 10000 !5000   !1000
      n_skip  = 500 !100 !50
c-----------------------------------------
      call get_grid

      call calc_rci(curdir)  ! calculate lambda_ci

      stop
      end

c-------------------------------------------------------------------
      subroutine get_grid
      include 'param.h'
      common/mesh/y(nyp),dx,dz
      common/domain/sx,sz
      common/para/re

      pi = acos(-1.0)
      do j=1,nyp
         y(j) = 1.0-cos(pi*real(j-1)/real(nyp-1))
      enddo

      dx = sx/real(nx)
      dz = sz/real(nz)

      return
      end

c-------------------------------------------------------------------
      subroutine calc_rci(curdir)
      include 'param.h'

      common/mesh/y(nyp),dx,dz
      common/domain/sx,sz
      common/para/re
      common/nstep/n_start, n_final, n_skip
      character*50 filename
      character*30 :: curdir
      real*8 d11(nx,nyp,nz),d12(nx,nyp,nz),d13(nx,nyp,nz)
      real*8 d21(nx,nyp,nz),d22(nx,nyp,nz),d23(nx,nyp,nz)
      real*8 d31(nx,nyp,nz),d32(nx,nyp,nz),d33(nx,nyp,nz)
      real*8 q1(nx,nyp,nz)
      real*8 q2(nx,nyp,nz)
      real*8 q3(nx,nyp,nz)
      real*8 uf(nx,nyp,nz)
```

```
      real*8 e11,e12,e13,e21,e22,e23,e31,e32,e33
      real*8 p,q,r,q0,r0,dis,reg1,reg2,reg3
      real*8 p_max
      real*8 ramda_ci(nx,nyp,nz)
      real*8 r_ci_max
c
      real*8 q1_xz(nyp)
      real*8 q2_xz(nyp)

c     TECPLOT STUFF
      integer  i,j,k,imax,jmax,kmax
      integer  debug,ier,itot
      integer  tecini,tecdat,teczne,tecnod,tecfil,tecend
      integer  visdouble,disdouble
      character*1 nulchar

      real*8 xt(nx,nyp,nz)
      real*8 yt(nx,nyp,nz)
      real*8 zt(nx,nyp,nz)

      nulchar = char(0)
      debug   = 0
      visdouble = 0
      disdouble = 1
      imax = nx
      jmax = nyp
      kmax = nz


        do 90 k=1,nz
        do 90 j=1,nyp
        do 90 i=1,nx
c---  with Fortran 90 we can just fill the arrays...
        xt(i,j,k) = real(i-1)*dx*re
        yt(i,j,k) = y(j)*re
        zt(i,j,k) = real(k-nz/2)*dz*re
90      continue

c
      do ntime=n_start,n_final,n_skip
c
         call get_vel(q1,q2,q3,ntime,curdir)

c
c--- read dij
        call get_filename_dij(filename,ntime,1,1,curdir)
        write(*,*) filename
        open(10,file=filename,status='old',form='unformatted'
     &         ,action='read')
        read(10) (((d11(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
        close(10)
        call get_filename_dij(filename,ntime,1,2,curdir)
        write(*,*) filename
        open(10,file=filename,status='old',form='unformatted'
     &         ,action='read')
```

```
   read(10) (((d12(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,1,3,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d13(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,2,1,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d21(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,2,2,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d22(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,2,3,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d23(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,3,1,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d31(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,3,2,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d32(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)
   call get_filename_dij(filename,ntime,3,3,curdir)
   write(*,*) filename
   open(10,file=filename,status='old',form='unformatted'
&         ,action='read')
   read(10) (((d33(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
   close(10)

 ramda_ci(:,:,:) = 0.0d0 ! ramda_ci

 do 1 j=1,nyp
 do 1 k=1,nz
 do 1 i=1,nx
    e11 = d11(i,j,k)
    e12 = d12(i,j,k)
    e13 = d13(i,j,k)
    e21 = d21(i,j,k)
    e22 = d22(i,j,k)
```

```
          e23 = d23(i,j,k)
          e31 = d31(i,j,k)
          e32 = d32(i,j,k)
          e33 = d33(i,j,k)
          p = - (e11 + e22 + e33)
          q = 0.5*(p**2 - (
     &                   +e11**2
     &                   +e22**2
     &                   +e33**2
     &                   +e12*e21*2.0
     &                   +e13*e31*2.0
     &                   +e23*e32*2.0
     &                    )
     &             )
          r = -( - e13*e22*e31 + e12*e23*e31
     &           + e13*e21*e32 - e11*e23*e32
     &           - e12*e21*e33 + e11*e22*e33
     &          )
          if (abs(p).gt.p_max) then
              p_max = abs(p)
          endif
          r0 = r + 2./27.*p**3 - 1./3.*p*q
          q0 = q - 1./3. *p**2
          dis = (r0/2.)**2 + (q0/3.)**3
          if (dis.gt.0.0) then
             reg1 = sqrt(dis)
             reg2 = reg1 - r0/2.0
             reg3 = reg1 + r0/2.0
             if (reg2 .gt. 0.0) then
                 reg2 = reg2**(1./3.)
             else
                 reg2 = -(-reg2)**(1./3.)
             endif
             if (reg3 .gt. 0.0) then
                 reg3 = reg3**(1./3.)
             else
                 reg3 = -(-reg3)**(1./3.)
             endif
             ramda_ci(i,j,k) = sqrt(3.)/2.0*(reg2 + reg3)
          else
             ramda_ci(i,j,k) = 0.0
          endif
 1     continue
       write(*,*) 'maximum du_i/dx_i*h/u_tau =',p_max

c---   find the maximum r_ci

         r_ci_max = 0.0

         do k=1,nz
         do j=1,nyp
         do i=1,nx
            r_ci_max = amax1(r_ci_max,ramda_ci(i,j,k))
         enddo
         enddo
```

```
        enddo

c        write(*,*) r_ci_max

!        filename='rci'
!        nn=index(filename,'i')
!        write(unit=filename(nn+1:),fmt='(bn,i5.5)') ntime
!        write(*,*) filename
!        open(10,file=filename,status='unknown')
!c        write(10,*) 'zone i=',nx,',j=',nyp/2+1
!c     &             ,',k=',nz/4*3-nz/4+1,',f=point'
!
!        filename='rss'
!        nn=index(filename,'s')
!        write(unit=filename(nn+2:),fmt='(bn,i5.5)') ntime
!        write(*,*) filename
!        open(13,file=filename,status='unknown')
!c        write(13,*) 'zone i=',nx,',j=',nyp/2+1
!c     &             ,',k=',nz/4*3-nz/4+1,',f=point'
!
!        filename='xy'
!        nn=index(filename,'y')
!        write(unit=filename(nn+1:),fmt='(bn,i5.5)') ntime
!        write(*,*) filename
!        open(11,file=filename,status='unknown')
!c        write(11,*) 'zone i=',nx,',j=',nyp/2+1
!c     &             ,',k=',1,',f=point'
!
!        filename='xy_uf'
!        nn=index(filename,'f')
!        write(unit=filename(nn+1:),fmt='(bn,i5.5)') ntime
!        write(*,*) filename
!        open(12,file=filename,status='unknown')
!c        write(12,*) 'zone i=',nx,',j=',nyp/2+1
!c     &             ,',k=',1,',f=point'

c---  calculate x-z mean of u and fpi

            q1_xz(:) = 0.0
            q2_xz(:) = 0.0
      do j = 1, nyp
         do k = 1, nz
         do i = 1, nx
            q1_xz(j) = q1_xz(j) + q1(i,j,k)/real(nx*nz)
            q2_xz(j) = q2_xz(j) + q2(i,j,k)/real(nx*nz)
         enddo
         enddo
      enddo

      do j = 1, nyp
         uf(:,j,:) = q1(:,j,:) - q1_xz(j)
      end do
c---

        do 2 k=nz/4,nz/4*3
```

```
        do 2 j=1,nyp/2+1
        do 2 i=1,nx
           rx=real(i-1)*dx*re
           rz=real(k-nz/2)*dz*re
           ry=y(j)*re

c           write(10,100) rx,ry,rz,ramda_ci(i,j,k)
c           write(13,100) rx,ry,rz,
c     &          (q1(i,j,k)-q1_xz(j))*(q2(i,j,k)-q2_xz(j))

           if( k .eq. nz/2 )  then
               rz2=real(nz/4-nz/2)*dz*re
c               write(11,101) rx,ry,rz2
c     &                       ,q1(i,j,k)- 0.8*q1_xz((nyp+1)/2)    !-
0.8*20.157  ! substract 80% centerline velocity
c     &                       ,q2(i,j,k)
c     &                       ,q3(i,j,k)
c!     &                       ,0.0

c               write(12,100) rx,ry,rz2
c     &                       ,q1(i,j,k)- q1_xz(j) ! substract xz mean
velocity
           endif

 2      continue

 100       format(4(e12.5,x))
 101       format(6(e12.5,x))
!        close(10)
!        close(11)
!        close(12)
!        close(13)

c---  TECPLOT output
        filename='./datatecplot/data'//trim(curdir)//'/chvfld@'
        nn=index(filename,'@')
        write(unit=filename(nn:),fmt='(bn,i5.5)') ntime
        write(*,*) trim(filename)
        filename = trim(filename)//'@'
        nn=index(filename,'@')

      ier = tecini('Velocity Field'//nulchar,
     &             'x,y,z,u,v,w,ufluc,dudx,dudy,dudz,dvdx,
     &             dvdy,dvdz,dwdx,dwdy,dwdz,lambdaci'//nulchar,
     &             filename(1:(nn-1))//'.plt'//nulchar,
     &             '.'//nulchar,
     &             debug,visdouble)


      !
      ! Write the zone header information.
      !
      ier = teczne('Velocity Field'//nulchar,
     &             imax,jmax,kmax,
     &             'BLOCK'//nulchar,nulchar)
```

```
      !
      ! Write out the field data.
      !
      itot = imax*jmax*kmax
      ier = tecdat(itot,xt,disdouble)
      ier = tecdat(itot,yt,disdouble)
      ier = tecdat(itot,zt,disdouble)
      ier = tecdat(itot,q1,disdouble)
      ier = tecdat(itot,q2,disdouble)
      ier = tecdat(itot,q3,disdouble)
      ier = tecdat(itot,uf,disdouble)
      ier = tecdat(itot,d11,disdouble)
      ier = tecdat(itot,d12,disdouble)
      ier = tecdat(itot,d13,disdouble)
      ier = tecdat(itot,d21,disdouble)
      ier = tecdat(itot,d22,disdouble)
      ier = tecdat(itot,d23,disdouble)
      ier = tecdat(itot,d31,disdouble)
      ier = tecdat(itot,d32,disdouble)
      ier = tecdat(itot,d33,disdouble)

      ier = tecdat(itot,ramda_ci,disdouble)

      ier = tecend()

      enddo ! ntime



      return
      end

c-----------------------------------------------------------------------
        subroutine get_vel(u,v,w,ntime,curdir)
        include 'param.h'

      character*30 :: curdir

        real*8 u(nx,nyp,nz)
        real*8 v(nx,nyp,nz)
        real*8 w(nx,nyp,nz)

        character*50 filename


c---  read u

        call get_filename_disk5(filename,ntime,1,curdir)
        write(*,*) filename
        open(10,file=filename,status='old',form='unformatted'
     &         ,action='read')
        read(10) (((u(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
        close(10)
```

```
c---  read v

        call get_filename_disk5(filename,ntime,2,curdir)
        write(*,*) filename
        open(10,file=filename,status='old',form='unformatted'
     &         ,action='read')
        read(10) (((v(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
        close(10)

c---  read w

        call get_filename_disk5(filename,ntime,3,curdir)
        write(*,*) filename
        open(10,file=filename,status='old',form='unformatted'
     &         ,action='read')
        read(10) (((w(i,j,k),i=1,nx),j=1,nyp),k=1,nz)
        close(10)


        return
        end

!c-------------------------------------------------------------------
!        subroutine get_filename_disk5(filename,ntime,nv)
!c       nv=1 : u
!c          2 : v
!c          3 : w
!
!        character*50 filename
!
!        filename='../../../scratch/data_vel/'
!        nn=index(filename,'/')
!        if (nv.eq.1) write(unit=filename(nn+10:),fmt='(bn,a5)')
'u1.00'
!        if (nv.eq.2) write(unit=filename(nn+10:),fmt='(bn,a5)')
'u2.00'
!        if (nv.eq.3) write(unit=filename(nn+10:),fmt='(bn,a5)')
'u3.00'
!        write(unit=filename(nn+15:),fmt='(bn,i5.5)') ntime
!
!        return
!        end

!c-------------------------------------------------------------------
      subroutine get_filename_disk5(filename,iseq,nv,curdir)
!c       nv=1 : u
!c          2 : v
!c          3 : w

      implicit none
      character*50 filename
      integer iseq, nv, nn
      character*30 curdir

      if (nv.le.4) then
```

```
      !filename='../data_vel/@'
      filename='../../../scratch/data_vel'//trim(curdir)//'/@'  !
directory where DNS results are stored.
      nn=index(filename,'@')
      if (nv.eq.1) write(unit=filename(nn:),fmt='(bn,a3)') 'u1.'
      if (nv.eq.2) write(unit=filename(nn:),fmt='(bn,a3)') 'u2.'
      if (nv.eq.3) write(unit=filename(nn:),fmt='(bn,a3)') 'u3.'
      if (nv.eq.4) write(unit=filename(nn:),fmt='(bn,a3)') 'pp.'
      write(unit=filename(nn+3:),fmt='(bn,i7.7)') iseq
      endif

        return
        end

!c-------------------------------------------------------------------
!      subroutine get_filename_dij(filename,iseq,nv1,nv2)
!!c       nv1=1 : u  nv2 = x
!!c       nv1=2 : v  nv2 = y
!!c       nv1=3 : w  nv2 = z
!      implicit none
!      character*50 filename
!      integer iseq, nv1,nv2,nn
!      filename='../../../scratch/data_dij/d'
!      nn=index(filename,'/')
!      write(unit=filename(nn+11:),fmt='(bn,i1.1)') nv1
!      write(unit=filename(nn+12:),fmt='(bn,i1.1)') nv2
!      write(unit=filename(nn+13:),fmt='(bn,a1)') '.'
!      write(unit=filename(nn+14:),fmt='(bn,i7.7)') iseq
!      return
!      end

!c-------------------------------------------------------------------
      subroutine get_filename_dij(filename,iseq,nv1,nv2,curdir)
!c       nv=1 : u
!c          2 : v
!c          3 : w

      implicit none
      character*50 filename
      integer iseq, nv1, nv2, nn
      character*30 curdir

      !if (nv.le.4) then
      !filename1='../data_dij/@'
      !filename2='../data_dij/@'
      !filename3='../data_dij/@'
      filename='../../../scratch/data_dij'//trim(curdir)//'/d@'  !
directory where DNS results are stored.
      nn=index(filename,'@')

      write(unit=filename(nn:),fmt='(bn,i1.1)') nv1
      write(unit=filename(nn+1:),fmt='(bn,i1.1)') nv2
      write(unit=filename(nn+2:),fmt='(bn,a1)') '.'
      write(unit=filename(nn+3:),fmt='(bn,i7.7)') iseq
```

```
!endif

return
end
```