Large eddy simulation of turbulent channel flow with buoyancy effects

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Large eddy simulation of turbulent channel flow
with buoyancy effects

by

Joon Sang Lee

A thesis submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of
MASTER OF SCIENCE

Major: Mechanical Engineering
Major Professor: Richard H. Pletcher

Iowa State University
Ames, Iowa
1999

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This is to certify that the Master’s thesis of
Joon Sang Lee
has met the thesis requirements of Iowa State University
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NOMENCLATURE

2CD  second order central differencing
rms  root-mean-square
DNS  direct numerical simulation
LES  large eddy simulation
RANS Reynolds-averaged Navier-Stokes equations
SGI  Silicon Graphic Inc.
SGS  subgrid scale

Roman Symbols

\( g \)  gravitational force
\( k \)  thermal conductivity
\( m \)  pseudo (local) time index
\( n \)  physical time index
\( \vec{\mathbf{\eta}} \)  unit normal vector
\( p \)  pressure
\( u_i \)  index notation for velocity
\( u_\tau \)  friction velocity \((=\sqrt{\tau_{wall}/\rho_{wall}})\)
\( u_\tau^* \)  \( \sqrt{\tau_{wall}/\rho(y)} \)
\( u^+ \)  \( u^*/u_\tau \)
\( y^+ \)  coordinate in wall units
\( \mathbf{B}, \vec{\mathbf{B}} \)  scalar and vector source term
\( C_d \)  coefficient from the dynamic SGS model
\begin{align*}
C_p & \quad \text{specific heat at constant pressure} \\
E_c & \quad \text{Eckert number} \\
F_l & \quad \text{forcing function} \\
F_r & \quad \text{Froude number} \\
[I] & \quad \text{identity matrix} \\
Ma & \quad \text{Mach number} \\
Pr & \quad \text{Prandtl number} \\
Pr_t & \quad \text{turbulent Prandtl number} \\
W & \quad \text{primitive variable vector} \\
R & \quad \text{gas constant} \\
\vec{R} & \quad \text{residual vector} \\
Ra & \quad \text{Rayleigh number} \\
Re & \quad \text{Reynolds number based on the initial velocity} \\
Re_\tau & \quad \text{friction Reynolds number, } u_\tau \delta / \nu \\
Re_m & \quad \text{bulk Reynolds number, } u_m \delta / \nu \\
Ri & \quad \text{Richardson number, } Gr / Re_m^2 \\
S_{ij} & \quad \text{rate of strain tensor} \\
T & \quad \text{thermodynamic temperature} \\
T^+ & \quad Pr y^+ \\
T^* & \quad T^+ \sqrt{P(y) / \rho_{\text{wall}}} \\
T_{\text{ref}} & \quad \text{reference temperature} \\
T_w & \quad \text{wall temperature} \\
T_\tau & \quad \text{friction temperature, } \frac{\tilde{\psi}_w}{\rho_0 c_p u_\tau} \\
U_c & \quad \text{channel centerline velocity} \\
\end{align*}

\textbf{Greek Symbols}

\begin{align*}
\alpha & \quad \text{thermal diffusivity} \\
\delta & \quad \text{channel half width}
\end{align*}
\[ \epsilon \]  temperature difference parameter
\[ \gamma \]  specific heat ratio
\[ \mu, \nu \]  dynamic and kinematic viscosity
\[ \mu_t \]  SGS eddy viscosity
\[ \rho \]  density
\[ \tau \]  pseudo time
\[ \tau_{wall} \]  local shear stress

**Subscripts**

\( i, j, k \)  indices in x, y, z directions
\( 0 \)  reference value at the standard atmospheric condition
\( h, c \)  hot and cold wall

**Superscripts**

\( ()^* \)  dimensional quantities
\( \hat{()} \)  Farve-averaged quantities
\( ()' \)  SGS turbulent fluctuation quantities
\( ()'' \)  resolvable turbulent fluctuation quantities
Structured grid finite volume formulations have been developed to solve the compressible Navier-Stokes equations for performing large eddy simulation of turbulent flows. These compressible formulations were developed using low Mach number preconditioning. Time marching was done with a coupled strongly implicit scheme. The discretization schemes were second-order accurate central difference and third-order accurate upwind and a comparison was made between two schemes. Validations were performed using turbulent compressible benchmark flows with low heat transfer. The results were compared to direct numerical simulation, experimental, and other large eddy simulation results. The large eddy simulations yielded excellent agreement with the direct numerical simulation and experimental results for incompressible turbulence. For the significant property variations, high heat transfer rate was imposed and the effects of buoyancy on the turbulent structures under stably, and unstably stratified flows were investigated. The effects of buoyancy were larger in the central region of channel where the largest Richardson number occurred. Despite the fact that the relative buoyancy production was small near the boundary walls, effects of buoyancy were observed.
1 OVERVIEW

1.1 Overview

Turbulent flow occurs in many engineering applications. In the past, analysis of the turbulent structure has been difficult, and it has been almost impossible to measure all the important values experimentally. However, it is possible with computer simulations to view the flow variables in three-dimensional space. Before the computational method is introduced in this chapter, it is necessary to define turbulence in order to understand the objective of this project and its goals. Turbulence is characterized by the following words:

- Turbulent flows are unpredictable in the sense that small uncertainties in initial conditions leads to exponentially increasing uncertainties in future particle trajectories. In other words, turbulent flows are chaotic.
- Turbulent flows have highly increased mixing properties.
- Turbulent flows involve a wide range for spatial and temporal scales. They are threedimensional and time dependent.

According to Hinze (1975, p2), the above definition can be summarized as follows, “Turbulent fluid motion is an irregular condition of flow in which the various quantities show a random variation with time and space coordinates so that statistically distinct average values can be discerned.”

Generally, turbulent fluid motion is governed by the unsteady Navier-Stokes (N-S) equations. Even if basic conservation concepts (conservation of mass, momentum, and energy) are enforced by the N-S equations, there is no analytical solution available. Numerical approaches are adopted to overcome this difficulty, but still getting accurate solutions is quite a challenge.
1.1.1 Direct Numerical Simulation (DNS)

Direct numerical simulation (DNS) refers to solving the N-S equations without averaging or approximation except for the numerical discretization. It, therefore, attempts to resolve all the motions from largest to smallest scales. Since all the scales need to be resolved, grids should be very fine to capture all the small scales. Moin (1984) approximated the relation between grid points and mean Reynolds number,

\[ N \simeq (3Re_m)^{\frac{5}{4}} \]  

(1.1)

where \( Re_m \) is the Reynolds number based on the mean velocity.

As it can be seen, the required number of gridpoints is proportional to the \( \frac{5}{4} \) power of the \( Re_m \). Since the number of gridpoints is limited by computational speed and memory, today, DNS can be performed at low Reynolds numbers (Re) only.

Another requirement is that DNS should be performed with high-order accurate schemes in order to use a relatively coarse grid size, but it still requires large computational resources. Despite the large computer resources required, many researchers (Kim at al., 1987; Reynolds, 1990; Kasagi et al., 1998; Debusschere et al., 1998) have used this method, and have shown it to be a valuable tool to predict flow and heat transfer characteristics. The information obtained on velocity, pressure and temperature may be regarded as the equivalent of experimental data or as even more accurate than some experimental data. For instance, Kim et al. (1987) have pointed to some possible errors of standard hot-wire techniques after some discrepancies were found between their computational data and reference experimental data.

In short, DNS is clearly able to provide very accurate data, and it is an attractive approach if there are enough resources available. However, it is not feasible to use DNS for flows in which the Reynolds number is too high or the geometry is too complex.

1.1.2 Large Eddy Simulation (LES)

As explained, DNS requires high-order numerical schemes and still a fine grid to resolve all the scales of motion; besides, it requires a huge amount of computational resources. Unlike
DNS, large eddy simulation (LES) doesn't attempt to resolve all scales; rather, it only resolves the large scale motions.

In term of strength, the small scales are much weaker and provide little transport to the conserved properties. They can be considered as nearly isotropic in the LES method. These small scale motions are filtered out and their effects only represented using a “subgrid scale” (SGS) model. Since only large scale motions are resolved, LES uses fewer computational resources making it more appropriate for more complex flows than can be addressed by DNS.

Recently, the most widely used SGS models have been the Smagorinsky (Smagorinsky, 1963), and dynamic (Germano et al., 1990) models. The basic difference between the two models is that dynamic model is able to evaluate the proportionality of the model constant at every spatial gridpoint and time step by use of the LES results. For instance, the effect of the model has to be reduced very near the wall. The dynamic model correctly reduces the parameter whereas _ad hoc_ damping needs to be employed with the Smagorinsky model. However, in its present state, the spatial variations in the model parameters predicted by the dynamics model may cause numerical stability problems for some schemes.

### 1.1.3 Reynolds Averaged Navier-Stokes (RANS) Method

Methods such as DNS and LES require enormous computer resources and provide information with more detail than is necessary for many applications. This is why the Reynolds averaged Navier-Stokes (RANS) method is most commonly used in the CFD community. “Averaged” means that all the unsteadiness is averaged out by use of time averaging. Initially, all the variables are defined as

\[
\phi(x_i, t) = \bar{\phi}(x_i) + \phi'(x_i, t)
\]

where \( \bar{\phi}(x_i) = \lim_{T \to \infty} \frac{1}{T} \int_0^T \phi(x_i, t)dt \), \( t \) is the time and \( T \) is the averaging interval.

On averaging, the character of nonlinearity needs to be treated specially, i.e., needs to be modeled. Various modeling has been used among researchers and the degree of success has been varied, as well.
In spite of many efforts to develop turbulence models, the progress has been limited so far. The large scales depend, as mentioned before, more on geometry and it is, therefore, not appropriate to apply RANS which models all the scales in many applications. DNS and LES methods are gaining popularity in the CFD community as a means to overcome the difficulties associated with the RANS method.

1.2 Goals of the Present Study

In the design of engineering applications like aircraft, vehicles, and internal combustion engines, accurate predictions of turbulent flow are needed. Without using accurate methods, predicting and understanding the complex flows and engineering applications are impossible.

In the past, many turbulent flows have been analyzed experimentally. As computer power and speed have increased and better and better numerical schemes developed, researchers have attempted to solve the turbulent flows numerically using the models (RANS, DNS, LES) described above.

The present research is concerned with turbulent channel flow with heat transfer. Effects of buoyancy and property variations are to be considered. Scalar transport in turbulent channel flows has been studied by Kim and Moin (1989) using DNS. Wang and Pletcher (1994) performed LES of compressible turbulent flows which permitted large variation in fluid properties. Two different isothermal wall boundary conditions were used for the top and bottom walls. Results showed the minimum velocity fluctuations at the center because there was no mean velocity gradient at that location. Unlike velocity fluctuations, the maximum temperature fluctuations were found at the center of channel. Since there is energy transfer from the heated to the cooled wall, the whole domain contains temperature gradients including the center of the channel.

Since the top and bottom wall temperatures were significantly different, Nicoud and Poinrot (1999) observed different local values of Reynolds number near the wall in their DNS results. The higher Reynolds number was observed near cold wall and lower one found near the hot wall. The variations in Reynolds number were thought to be responsible for a variation in the
size of the turbulent structures. The structures near the hot wall were much larger than values near the cold wall. These different Reynolds numbers were obviously due to different density and viscosity values which were functions of temperature.

Some experimental studies have been conducted to reveal the effects of buoyancy near the wall (Kasagi and Hirata, 1977; Mizushima et al., 1982; Fukui and Nakajima, 1985) in turbulent channel flow. These researchers found that unstably stratified flow influenced structures differently in the central and wall regions. Recently, Kasagi and Iida. (1998) performed DNS of buoyancy effects on turbulent transport in the horizontal channel flow and pointed out that Reynolds stress caused some alternation in the turbulent structures which mainly contributed by thermal plumes.

In this research, an LES study of a fully developed horizontal channel flow with property variations at low and high boundary wall temperature ratios were performed and buoyancy effects on turbulent structures in the near wall and central region of the channel were investigated. Since Kasagi and Iida. (1998) have investigated a similar buoyancy condition for incompressible flow, it will be of interest to make comparison with the current compressible case. This study will provide more reliable data about variable property case with buoyancy effects to the turbulent structures.

1.3 Outline of the Thesis

Chapters 2 and 3 discuss the filtering operation of the compressible Navier-Stokes (N-S) equations, and the finite volume formulation. The dynamic subgrid scale (SGS) model is to be discussed in chapter 3.

Chapter 4 gives the results of the isothermal wall channel flow with buoyancy. Results with low heat transfer using the central and upwind schemes, and with high heat transfer for the stable and unstable buoyancy cases will be given. Direct numerical simulations, large eddy simulations, and experimental data are used to make comparisons with results from this study.

Chapter 5 will summarize the present work along with conclusions, and recommendations for the future research.
2 FILTERING OPERATION OF COMPRESSIBLE N-S EQUATIONS

In this chapter, the fully compressible N-S equations are to be introduced and the compressible dynamic SGS model discussed. For gas flow with property variations (density, viscosity, and thermal conductivity), the compressible N-S equations need to be employed even if the low speed case is dealt with.

2.1 Compressible Nondimensional Navier-Stokes (N-S) Equations

The equations of fluid dynamics are fundamentally based on the following three conservation laws:

- Conservation of mass

\[
\frac{\partial \rho^*}{\partial t^*} + \frac{\partial (\rho^* u_i^*)}{\partial x_i^*} = 0 \tag{2.1}
\]

- Conservation of momentum

\[
\frac{\partial (\rho^* u_i^*)}{\partial t^*} + \frac{\partial (\rho^* u_i^* u_j^*)}{\partial x_j^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{\partial \sigma_{ij}^*}{\partial x_j^*} + F_i^* \delta_{1i} - \rho^* g \delta_{2i} \tag{2.2}
\]

- Conservation of energy

\[
\frac{\partial (\rho^* C_p T^*)}{\partial t^*} + \frac{\partial (\rho^* u_i^* C_p T^*)}{\partial x_j^*} = \frac{\partial p^*}{\partial t^*} + u_j^* \frac{\partial p^*}{\partial x_j^*} + \sigma_{ij}^* \frac{\partial u_i^*}{\partial x_j^*} - \frac{\partial q_i^*}{\partial x_i^*} \tag{2.3}
\]

where the dimensional variables are denoted by an asterisk. \( F_i^* \) represents a mean pressure gradient, and the last term of Eq. (2.2) is the gravitational term. The dimensional viscous stress and heat flux terms appearing in Eq. (2.3) are
\[
\sigma_{ij}^* = \mu^* \left( \frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} \right) + \lambda^* \frac{\partial u_k^*}{\partial x_k^*} \delta_{ij} \tag{2.4}
\]

\[
q_j^* = -k^* \frac{\partial T^*}{\partial x_j^*} \tag{2.5}
\]

where \( \mu^* \) is the dynamic viscosity, \( \lambda^* \) is the bulk viscosity (\( \approx -2/3 \mu^* \)), and \( k^* \) is the thermal conductivity.

A perfect gas equation of state is used since the intermolecular forces are assumed to be negligible,

\[
p^* = \rho^* R^* T^* \tag{2.6}
\]

where \( R^* \) is the dimensional gas constant. For the property evaluations, the following functions are used,

\[
\frac{\mu^*}{\mu_0} = \left( \frac{T^*}{T_0} \right)^a \tag{2.7}
\]

\[
\frac{k^*}{k_0} = \left( \frac{T^*}{T_0} \right)^a \tag{2.8}
\]

where the subscript 0 denotes the reference state values. The superscript \( a \) has been taken as 0.71.

The above dimensional N-S equations are to be non-dimensionalized to take advantage of characteristic parameters and normalized variables. The nondimensional variables are defined as follows,

\[
x_i = x_i^* / L_0 \quad u_i = u_i^* / U_0 \quad t = t^* / L_0 / U_0 \tag{2.9}
\]

\[
\rho = \rho_i^* / \rho_0 \quad p = p_i^* / \rho_0 U_0^2 \quad F_1 = F_i^* / \rho_0 U_0^2 L_0 \tag{2.10}
\]

\[
\mu = \mu_i^* / \mu_0 \quad k = k_i^* / k_0 \quad T = T^* - T_0 / T_{ref} \tag{2.11}
\]

\[
R = 1/\gamma M_0^2 \tag{2.12}
\]
where the subscript 0 denotes values at a reference state. \( L_0, U_0, \rho_0, \) and \( T_0 \) are the channel half width, initial centerline velocity, density, and temperature, respectively. \( T_{\text{ref}} = \frac{1}{2}(T_{\text{bottom}} - T_{\text{top}}) \)

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \tag{2.13}
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + F_i \delta_{ij} - \frac{1}{F_r^2} \rho \delta_{2i} \tag{2.14}
\]

\[
\frac{\partial (\rho T)}{\partial t} + \frac{\partial (\rho u_j T)}{\partial x_j} = E_c (\frac{\partial p}{\partial t} - u_j \frac{\partial p}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j}) - \frac{\partial q_i}{\partial x_i} \tag{2.15}
\]

where the Eckert number, \( E_c \), is,

\[
E_c = \frac{U_o^2}{C_p T_{\text{ref}}} \tag{2.16}
\]

the non-dimensional heat flux vector is,

\[
q_j = -\frac{k}{PrRe} \frac{\partial T}{\partial x_j} \tag{2.17}
\]

the dimensionless viscous stress term, \( \sigma_{ij} \), is,

\[
\sigma_{ij} = \mu (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) + \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij} \tag{2.18}
\]

and the Froude number, \( Fr \), is,

\[
F_r = \frac{u}{\sqrt{gL_0}} \tag{2.19}
\]

The Eckert number is expected to be very small for the subsonic flows encountered in the current investigation, so the term containing it will be neglected in Eq. 2.15.
2.2 Filtering

To separate the large-scale (or resolved) variables, denoted by an over bar, from the small-scale variables, a filtering operation needs to be defined as

$$\tilde{f}(x) = \int_D f(x')G(x,x')dx'$$  \hfill (2.20)

where $G$ is the filter function, and $D$ is the entire domain.

There are three different forms of the filter function have been used in CFD applications, and they are the spectral cut-off, Gaussian, and top-hat functions. In this research, the top-hat function were used, and it is defined as

$$G(x) = \begin{cases} 1/\Delta & \text{if } |x| \leq \Delta/2 \\ 0 & \text{otherwise} \end{cases}$$  \hfill (2.21)

where $\Delta$ is the filter width given by $\Delta = (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}}$. $\Delta_x$, $\Delta_y$, and $\Delta_z$ are the control volume dimensions in the x, y, and z directions.

2.3 Mass-Weighted (Favre) Averaging

The unsteady compressible N-S equations are a mixed set of hyperbolic-parabolic equations in time, and it is possible to solve them for both low and high speed flow cases. However, the treatment of compressibility is not convenient unless mass-weighted averaging is used. Much of the development of the filtering operation follows that of Simons (1998). To simplify the filtered equations, a Farve-averaging (Erlebacher et al. 1990) is applied. This mass-weighted approach introduces the following new variables.

$$\tilde{f} = \frac{\rho \tilde{f}}{\rho}$$  \hfill (2.22)

where $f$ is a general flow variable.

Generally, the variable can be decomposed as

$$f = \tilde{f} + f'$$  \hfill (2.23)
where $\tilde{f}$ and $\tilde{f}'$ are the Favre-averaging variables and its fluctuation, respectively.

The compressible N-S equation, Eq 2.13 - 2.15, are filtered and become

$$\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_i)}{\partial x_j} = 0$$  \hspace{1cm} (2.24)

$$\frac{\partial (\tilde{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_i \tilde{u}_j)}{\partial x_j} = - \frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + F_i \delta_{1i} - \frac{1}{Fr^2} \tilde{\rho} \delta_{2i} \frac{\partial \tau_{ij}}{\partial x_j}$$  \hspace{1cm} (2.25)

$$\frac{\partial (\tilde{\rho} \tilde{T})}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_j \tilde{T})}{\partial x_j} = - \frac{\partial q_{ij}}{\partial x_j} - \frac{\partial q_{i,j}}{\partial x_j}$$  \hspace{1cm} (2.26)

where the filtered viscous stress tensor is

$$\sigma = \mu \text{Re} \left[ \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \sigma_{ij} \right]$$  \hspace{1cm} (2.27)

the turbulent stress tensor and heat flux vector are

$$\tau_{ij} = \tilde{\rho} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j)$$  \hspace{1cm} (2.28)

$$q_{ij} = \rho \tilde{u}_j \tilde{T} - \tilde{u}_j \tilde{T}$$  \hspace{1cm} (2.29)

### 2.4 Dynamic Models

Dynamic modeling of the subgrid-scale stresses was introduced by Germano et al. (1991). Unlike the Smagorinsky model, the model coefficients, $C_d$ and $C_l$, are computed dynamically as the computation progresses. Before the dynamic model coefficients are introduced, a test filter should be given by

$$\hat{f}(x) = \int_D f(x') \hat{G}(x, x') dx'$$  \hspace{1cm} (2.30)

where $\hat{G}$ is the test filter that is two times larger than the filter function $G$. The dynamic model for this research was based on Wang’s (1995) derivation. By use of Lilly’s (1992) approach, the unknown parameters, $C_d$, and $C_l$ can be determined as
\[ C_d = \frac{-1}{2\Delta^2} \frac{\langle D_{ij}P_{ij} \rangle}{\langle P_{ij}P_{ij} \rangle} \]  
(2.31)

\[ C_l = \frac{-1}{\Delta^2} \frac{\langle \hat{\rho}\hat{u}_k\hat{u}_k - \langle \hat{\rho}\hat{u}_k\hat{u}_k \rangle \hat{\rho} \rangle}{\langle \hat{2}(\hat{\rho}\hat{T})^2 - \hat{\rho}\hat{T}^2 \rangle} \]  
(2.32)

where \( \langle \cdot \rangle \) denotes spatial averaging along the streamwise and spanwise directions of the flow, \( |S| \) is the magnitude of strain rate tensor, \( \Delta \) is the filtered width \( (= (\Delta_x \Delta_y \Delta_z))^{1/3} \), and \( \alpha \) is the strain grid ratio \( (= \Delta/\Delta) \). The superscripts(\( \cdot, \cdot \)) denote the nonlinear function of Favre filtered quantity, large scale component of filtered quantity, and large scale component of Favre filtered quantity, respectively. \( D_{ij} \) and \( P_{ij} \) are defined as

\[ D_{ij} = \frac{\langle \hat{\rho}\hat{u}_i\hat{u}_j - \langle \hat{\rho}\hat{u}_i\hat{u}_j \rangle \hat{\rho} \rangle}{\hat{\rho}} - \frac{1}{3} \langle T_{kk} - \tau_{kk} \rangle \delta_{ij} \]  
(2.33)

\[ P_{ij} = \hat{\rho}|S|[\langle \hat{S}_{ij} - \frac{1}{3} \hat{S}_{kk} \delta_{ij} \rangle - \langle \hat{\rho}\hat{T}\rangle [\langle \hat{S}_{ij} - \frac{1}{3} \hat{S}_{kk} \delta_{ij} \rangle]] \]  
(2.34)

The turbulent heat flux in the energy equation needs to be modeled, too. Again, most of derivation for the turbulent heat flux can be found in Wang (1995), and it is defined as

\[ q_{ij} = -\hat{\rho}\nu_H \frac{\partial \hat{T}}{\partial x_j} \]  
(2.35)

where the SGS eddy heat diffusivity is

\[ \nu_H = \frac{C_d \Delta^2}{Pr_t |\hat{S}_{ij}|} \]  
(2.36)

and the turbulent Prandtl number \( (Pr_t) \) is

\[ Pr_t = \frac{1}{C_d \Delta^2} \frac{\langle F_k F_k \rangle}{\langle E_k F_k \rangle} \]  
(2.37)

\( E_k \) and \( F_k \) are defined as

\[ E_k = \frac{1}{\hat{\rho}} \langle \hat{\rho}\hat{u}_k\hat{u}_k \hat{T} \rangle - \langle \hat{\rho}\hat{T}\rangle \]  
(2.38)
\[ F_k = \Delta_0^2 \rho |\mathcal{S}| \frac{\partial \bar{T}}{\partial x_k} - \Delta_0^2 \rho |\mathcal{S}| \frac{\partial \bar{T}}{\partial x_k} \]
3 FINITE VOLUME FORMULATION AND ITS DISCRETIZATION

A suitable approximating method must be chosen to represent the Navier-Stokes equations since the equations cannot be solved analytically. The most popular methods are finite difference, finite volume and finite element methods. No matter what type of discretization method is used, the final solution should be same if the grid is fine enough, but there are some advantages and disadvantages of the various methods depending on the physical and computational domains.

Here, the author chose the finite volume method because of its simplicity and flexibility. The further details are given below.

3.1 Finite Volume Approach and Vector Form of the Equations

The finite volume method can be used for discretization in a very flexible manner because the whole physical domain can be decomposed into an arbitrary number of subdomains as long as the subdomains fill the whole domain completely. Another advantage is that it directly applies the conservation laws into the physical system. Much of development of the present finite volume method follows that of Wang (1995), Simons (1998), and Dailey (1998).

The demonstration of the finite volume method can be shown by use of the general conservation equation in three dimensions.

$$\frac{\partial}{\partial t} U + \frac{\partial}{\partial x} E + \frac{\partial}{\partial y} F + \frac{\partial}{\partial z} G = B$$

(3.1)

The above equation can be integrated by

$$\frac{\partial}{\partial t} \int_{V} U dV + \int_{S} [E_{i} F_{j} G_{k}] \cdot dS = \int_{V} B dV$$

(3.2)
where $E$, $F$, and $G$ are flux vectors, $B$ is a general source term, $V$ is the volume, and $S$ is the surface area.

Two volume and one surface integrations need to be approximated (see Appendix A). The approximation for the volume integration is made by use of the mean value theorem as

$$\frac{\partial}{\partial t} \int_V U dV \approx (\frac{d}{dt} U)_{ijk} \Delta V_{i,j,k}$$

(3.3)

The surface integration is approximated using the mid-point rule.

$$\int_S [E_i F_j G_k] dS \approx \sum_{n=1}^{6} ((E + F + G) \cdot \Delta S)$$

(3.4)

where $n$ denotes the six faces of the control volume.

Finally, Eq 3.1 becomes

$$\frac{dU}{dt} \Delta V + \sum_{n=1}^{6} ((E + F + G) \cdot \Delta S) = B \Delta V$$

(3.5)

For the orthogonal, Cartesian grid control volume, the two face flux directions are all perpendicular to two cell faces and this leads to $\Delta V = \Delta x \Delta y \Delta z$, $\Delta S_x = \Delta y \Delta z$, $\Delta S_y = \Delta x \Delta z$, and $\Delta S_z = \Delta x \Delta y$ (in the $x$, $y$, $z$ directions, respectively). If Eq. 3.5 is divided by $\Delta V$, it becomes

$$\frac{dU}{dt} + \frac{1}{\Delta x} (E_{i+\frac{1}{2}} - E_{i-\frac{1}{2}}) + \frac{1}{\Delta y} (F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}) + \frac{1}{\Delta z} (G_{k+\frac{1}{2}} - G_{k-\frac{1}{2}}) = B$$

(3.6)

where subscript $i + \frac{1}{2}, i - \frac{1}{2}, j + \frac{1}{2}, j - \frac{1}{2}, k + \frac{1}{2},$ and $k - \frac{1}{2}$ denote evaluation at the cell bases as shown in Fig. 3.1.

### 3.2 Discretization Methods

The arrangement of a numerical grid can be either regular or staggered. A staggered grid is generally more difficult to implement in unstructured and/or non-orthogonal grids because each variable needs to have its own control volume (see Fig 3.2). Since the author is dealing with a three-dimensional case, there would need to be four control volumes associated with
each nodal points. A regular grid offers a significant advantage in complicated solution domains because it only requires one control volume per node for evaluation of all primitive variables. Since the use of the regular grid arrangement often leads to a decoupling of the pressure and velocity fields, the staggered arrangement has been the most widely used for LES to date.

A major advantage of the staggered grid arrangement is the strong coupling between the velocities and the pressure (Wang et al., 1994). This prevents oscillations in pressure and velocity. In this research, the author has used the staggered arrangement since the physical and computational domains are simple. By applying the above numerical grids, Eq. 3.6 becomes

\[
\frac{d\vec{W}}{dt} + \frac{1}{\Delta x}(\overline{E_{i+\frac{1}{2}}} - \overline{E_{i-\frac{1}{2}}}) + \frac{1}{\Delta y}(\overline{F_{j+\frac{1}{2}}} - \overline{F_{j-\frac{1}{2}}}) + \frac{1}{\Delta z}(\overline{G_{k+\frac{1}{2}}} - \overline{G_{k-\frac{1}{2}}}) = B 
\]

where

\[
\vec{W} = [\rho, \rho u, \rho v, \rho w, \rho T]^T
\]

If the fluxes are generalized as

\[
\vec{F} = \vec{F}^{inv} - \vec{F}^{vis}
\]

where subscripts inv, vis denote inviscid and viscous, respectively.
Figure 3.2 Staggered arrangement of velocity and pressure

\[
\begin{pmatrix}
\rho \vec{V} \\
\rho \vec{V}_u + p_i \\
\rho \vec{V}_v + p_j \\
\rho \vec{V}_w + p_k \\
p\vec{V}T \\
0 \\
(\sigma + \tau)_i \\
(\sigma + \tau)_j \\
(\sigma + \tau)_k \\
-\bar{q} + \bar{q}_t
\end{pmatrix}
\]

where

\[
q_{ij} = \frac{\mu}{Re} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \right) 
\]

(3.8)

\[
\tau_{ij} = \frac{1}{3} q^2 \delta_{ij} - 2 \nu_l (S_{ij} - \frac{1}{3} S_{kk} \delta_{ij}) 
\]

(3.9)

\[
\bar{q}_j = -\frac{k}{Pr Re} \frac{\partial T}{\partial x_j}
\]

(3.10)
\[
\bar{q}_{i,j} = -\frac{\rho v_t}{Pr_t} \frac{\partial T}{\partial x_j}
\]

(3.11)

\(Pr_t\) is the SGS turbulent Prandtl number, and \(v_t\) is the SGS eddy viscosity.

\[
B = \begin{bmatrix}
0 \\
F_i \\
-[Ra/(2\epsilon Pr Re^2)](p/T) \\
0 \\
-[Ra/(2\epsilon Pr Re^2)](pv/T)
\end{bmatrix}
\]

where \(Ra\) is the Rayleigh number, and \(\epsilon\) is the temperature difference parameter. They are defined by

\[
Ra = \frac{2\epsilon g \rho^2 \delta^3 Pr}{\mu^2}
\]

(3.12)

\[
\epsilon = \frac{T_h - T_c}{T_h + T_c}
\]

(3.13)

where \(h\) and \(c\) denote the hot and cold walls.

### 3.3 Preconditioning Method and Time Discretization for Compressible N-S Equations

Many compressible equations become very inefficient and sometimes very inaccurate at low Mach numbers. This is due to an ill-conditioned algebraic problem. In other words, the ratio of the acoustic speed to the convective speed becomes very large, and this makes the computation expensive (Volpe 1991). To remedy this, a pseudo-time term is added into each equation which has same form as the physical time term, but premultiplied by the dimensionless gas constant \(R\) in the first column of the pseudo time matrix as developed by Pletcher and Chen. (1993). By using this method, the ill-conditioned problem can be eliminated and the whole equation can be solved efficiently. This preconditioned formulation has been investigated by many researchers (Turkel, 1987; Feng and Merkle, 1990; Choi and Merkle, 1990; Pletcher and Chen, 1993), and it has proved to be effective over wide range of Mach numbers.
The pseudo and physical time terms are treated differently when they are discretized. Since the pseudo time term vanishes at convergence, accuracy is not important, rather, only speed of convergence. The first-order backward scheme was used in the pseudo time term and the second-order three-level implicit scheme was used in the physical time term.

\[
\frac{d\bar{W}}{d\tau} = \frac{\bar{W}^{n+1,m+1} - \bar{W}^{n+1,m}}{\Delta \tau} \quad (3.14)
\]

\[
\frac{d\bar{W}}{dt} = \frac{3\bar{W}^{n+1,m+1} - 4\bar{W}^{n} + \bar{W}^{n-1}}{2\Delta t} \quad (3.15)
\]

where superscripts \( n \) and \( m \) denote physical and pseudo time, respectively.

### 3.4 Flux Discretization

Discretizing the fluxes was somewhat more complicated than dealing with time terms. Fluxes were divided into inviscid and viscous terms, because they were discretized based on different concepts. The author has used both central and upwind schemes. Checking and comparing the accuracy has been completed and will be reported in chapter 4.

Upwind schemes have good stability properties even at high Reynolds numbers, but they are generally more complicated to implement than central difference schemes. In this research, the upwind scheme has been used for low, and high heat transfers cases and a central difference has been used only for the low heat transfer case. The accuracy of both schemes will be discussed later.

For viscous fluxes, a central difference scheme has been applied due to the elliptic nature of the viscous operator. The order of accuracy has been determined based on that of inviscid fluxes. For example, if second-order central difference is used in inviscid fluxes, the same order of accuracy is used for viscous fluxes which is

\[
\left( \frac{\partial u}{\partial x} \right)_{i+1/2,j,k} = \frac{u_{i+1,j,k} - u_{i,j,k}}{x_{i+1} - x_i} \quad (3.16)
\]

For the 3rd order upwind scheme, a fourth-order central difference was used. All the equations and derivations can be found in Wang (1995).
3.5 Linearization and Jacobian Matrices

For any implicit method as adopted by the author in this study, nonlinear terms appeared and they were linearized by a Newton’s method.

3.5.1 Example of 2-D Continuity Equation Discretization

The simple 2-D continuity equation is chosen to demonstrate the numerical discretization. Figure 3.3 shows the two-dimensional grid arrangement. Expanding from 2-D to 3-D is easy enough by adding the z-coordinate. All other equations, momentum and energy, are discretized in a very similar manner.

\[ \frac{\partial p}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0 \]  \hspace{1cm} (3.17)

Since \( \rho = p/RT \) from the ideal gas equation,

\[ \frac{\partial}{\partial t} \left( \frac{p}{RT} \right) + \frac{\partial}{\partial x_j} \left( \frac{p}{RT} u_j \right) = 0 \] \hspace{1cm} (3.18)

After the pseudo-time term is added, and multiplied by a constant R, the equation becomes
\[ \frac{\partial}{\partial x} \left( \frac{pR}{T} \right) + \frac{\partial}{\partial y} \left( \frac{pV}{T} \right) + \frac{\partial}{\partial x} \left( \frac{pU}{T} \right) + \frac{\partial}{\partial y} \left( \frac{pV}{T} \right) = 0 \] (3.19)

The third and fourth terms of the right hand side (RHS) of Eq 3.19 are integrated as given below.

\[ \int \int \frac{\partial}{\partial x} \left( \frac{pU}{T} \right) dx dy + \int \int \frac{\partial}{\partial y} \left( \frac{pV}{T} \right) dx dy = \left( \left( \frac{pU}{T} \right)_e - \left( \frac{pU}{T} \right)_w \right) \Delta y + \left( \left( \frac{pV}{T} \right)_n - \left( \frac{pV}{T} \right)_s \right) \Delta x \] (3.20)

After dividing by \( \Delta x \), \( \Delta y \), the RHS becomes

\[ \text{RHS} = \frac{1}{\Delta x} \left[ \left( \frac{pU}{T} \right)_e - \left( \frac{pU}{T} \right)_w \right] + \frac{1}{\Delta y} \left[ \left( \frac{pV}{T} \right)_n - \left( \frac{pV}{T} \right)_s \right] \] (3.21)

The first term on the right hand side of Eq. 3.21 is discretized by second order central differences.

\[ \frac{1}{\Delta x} \left( \frac{pU}{T} \right)_e = \frac{1}{\Delta x} \left[ (W_1)_r \left( \frac{pU}{T} \right)_{i+1,j}^{n+1,k+1} + (W_2)_r \left( \frac{pU}{T} \right)_{i,j}^{n+1,k+1} \right] \] (3.22)

where

\[ (W_1)_r = \frac{x f(i + 1) - x c(i)}{x c(i + 1) - x c(i)} \] (3.23)

and

\[ (W_2)_r = \frac{x c(i + 1) - x f(i)}{x c(i + 1) - x c(i)} \] (3.24)

Note that \( x f \) and \( x c \) denote face and center values.

Since the primitive values \((T, U, \text{and } p)\) are nonlinear, the Newton’s linearization is adopted.

\[ \frac{1}{\Delta x} \frac{pU}{T} = \frac{1}{\Delta x} \left( (W_1)_r \left( \frac{pU}{T} \right)_{i+1,j}^{n+1,k} + (W_1)_r \left( \frac{U}{T} \right)_{i+1,j}^{n+1,k} \Delta p + (W_1)_r \left( \frac{p}{T} \right)_{i+1,j}^{n+1,k} \Delta U + \right) \]
\[ (W_1)_r \left( \frac{pU}{T} \right)_{i+1,j}^{n+1,k} \Delta T + (W_2)_r \left( \frac{pU}{T} \right)_{i,j}^{n+1,k} + (W_2)_r \left( \frac{U}{T} \right)_{i,j}^{n+1,k} \Delta p + (W_2)_r \left( \frac{p}{T} \right)_{i,j}^{n+1,k} \Delta U + \]
\[ (W_2)_r \left( \frac{pU}{T} \right)_{i,j}^{n+1,k} \Delta T \] (3.25)

A similar concept applies to the second term of the right hand side of Eq. 3.21 as follows:
\[
\frac{1}{\Delta x} \frac{pU}{T} w = \frac{1}{\Delta x} ((W_1)_i \left( \frac{pU}{T}\right)_{i,j}^{n+1,k} + (W_1)_i \left( \frac{U}{T}\right)_{i,j}^{n+1,k} \Delta p + (W_1)_i \left( \frac{P}{T}\right)_{i,j}^{n+1,k} \Delta U +
(W_1)_i \left( \frac{pU}{T}\right)_{i,j}^{n+1,k} \Delta T + (W_2)_i \left( \frac{pU}{T}\right)_{i-1,j}^{n+1,k} + (W_2)_i \left( \frac{U}{T}\right)_{i-1,j}^{n+1,k} \Delta p + (W_2)_i \left( \frac{P}{T}\right)_{i-1,j}^{n+1,k} \Delta U +
(W_2)_i \left( \frac{pU}{T}\right)_{i-1,j}^{n+1,k} \Delta T)
\]

where

\[
W_1 = \frac{x f(i) - x c(i - 1)}{x c(i) - x c(i - 1)}
\]

and

\[
W_2 = \frac{x c(i) - x f(i)}{x c(i) - x c(i - 1)}
\]

The rest of the RHS terms can be discretized similarly.

The above linearization process, and procedures used in Wang (1995) result in the following equation.

\[
\frac{1}{\Delta t} [\Gamma] + \frac{1}{\Delta t} [T] \delta W + \sum_{k=1}^{6} \frac{1}{\Delta x_k} [([\bar{A}_{inv}] \cdot \bar{n}) + ([\bar{A}_{vis}] \cdot \bar{n})]_k^m \delta W_k = - \bar{R}
\]

where \( \delta W = W^{m+1} - W^m \). The superscript m denotes the pseudo time. The residual vector \( R \) can be found in Wang (1995).

**3.5.2 Jacobian Matrices**

The preconditioning matrix for the pseudo-time, \([\Gamma]\) is

\[
[\Gamma] = \begin{bmatrix}
\frac{1}{T_0} & 0 & 0 & 0 & -C \frac{p}{RT_0^2} \\
\frac{1}{T_0} u & \frac{p}{RT_0} & 0 & 0 & -C \frac{p}{RT_0^2} u \\
\frac{1}{T_0} v & 0 & \frac{p}{RT_0} & 0 & -C \frac{p}{RT_0^2} v \\
\frac{1}{T_0} \bar{u} & 0 & 0 & \frac{p}{RT_0} & -C \frac{p}{RT_0^2} w \\
\frac{1}{T_0} \bar{v} & 0 & 0 & 0 & \frac{p}{RT_0}
\end{bmatrix}
\]

(3.30)

The Jacobian matrix for the physical time \([T]\), inviscid vector \([\bar{A}_{inv}]\) and viscous vector \([\bar{A}_{vis}]\) can be shown as
\[ [T] = \begin{bmatrix}
\frac{1}{RT_0} & 0 & 0 & -C\frac{p}{RT_0^2} \\
\frac{1}{RT_0}u & \frac{p}{RT_0} & 0 & -C\frac{p}{RT_0^2}u \\
\frac{1}{RT_0}v & 0 & \frac{p}{RT_0} & -C\frac{p}{RT_0^2}v \\
\frac{1}{RT_0} & 0 & 0 & -C\frac{p}{RT_0^2} + \frac{p}{RT_0} \\
\end{bmatrix} \] (3.31)

\[ [A_{inv}]^\nu = \begin{bmatrix}
\frac{1}{RT_0}u & \frac{p}{RT_0} & 0 & 0 & -C\frac{p}{RT_0^2}u \\
\frac{1}{RT_0}u^2 & \frac{2p}{RT_0}u & 0 & 0 & -C\frac{p}{RT_0^2}u^2 \\
\frac{1}{RT_0}uv & \frac{p}{RT_0}v & \frac{p}{RT_0}u & -C\frac{p}{RT_0^2}uv \\
\frac{1}{RT_0}uw & \frac{p}{RT_0}w & 0 & \frac{p}{RT_0}u & -C\frac{p}{RT_0^2}uw \\
\frac{1}{RT_0}uT & \frac{p}{RT_0}T & 0 & 0 & -C\frac{p}{RT_0^2}u + \frac{p}{RT_0}u \\
\end{bmatrix} \] (3.32)

\[ [A_{inv}]^\nu = \begin{bmatrix}
\frac{1}{RT_0}v & 0 & \frac{p}{RT_0} & 0 & -C\frac{p}{RT_0^2}v \\
\frac{1}{RT_0}vu & \frac{p}{RT_0}v & \frac{p}{RT_0}u & -C\frac{p}{RT_0^2}uv \\
\frac{1}{RT_0}v^2 & 0 & \frac{2p}{RT_0}v & 0 & -C\frac{p}{RT_0^2}v^2 \\
\frac{1}{RT_0}vw & 0 & \frac{p}{RT_0}w & \frac{p}{RT_0}v & -C\frac{p}{RT_0^2}vw \\
\frac{1}{RT_0}vT & 0 & \frac{p}{RT_0}T & 0 & -C\frac{p}{RT_0^2}v + \frac{p}{RT_0}v \\
\end{bmatrix} \] (3.33)

\[ [A_{inv}]^\nu = \begin{bmatrix}
\frac{1}{RT_0}w & 0 & 0 & \frac{p}{RT_0} & -C\frac{p}{RT_0^2}w \\
\frac{1}{RT_0}wu & \frac{p}{RT_0}w & 0 & \frac{p}{RT_0}u & -C\frac{p}{RT_0^2}wu \\
\frac{1}{RT_0}wv & 0 & \frac{p}{RT_0}v & \frac{p}{RT_0}v & -C\frac{p}{RT_0^2}wv \\
\frac{1}{RT_0}w^2 & 0 & 0 & \frac{2p}{RT_0}w & -C\frac{p}{RT_0^2}w^2 \\
\frac{1}{RT_0}wT & 0 & 0 & \frac{p}{RT_0}T & -C\frac{p}{RT_0^2}w + \frac{p}{RT_0}w \\
\end{bmatrix} \] (3.34)
The implementation of the boundary conditions on the staggered grid requires special
treatment because it was forced to use fictitious points or "ghost" cells (see Fig. B.1). The
following boundary conditions were applied.

- zero normal pressure gradient
- no-slip tangential velocity
- isothermal wall
- periodic boundary at the inflow and outflow in the streamwise and spanwise directions
The ghost cell values were calculated by use of a three-point extrapolation (see Appendix B).
4 CHANNEL FLOW WITH LOW AND HIGH HEAT TRANSFER RATES AND BUOYANCY EFFECTS

The results for the isothermal wall case with heat transfer and buoyancy effects is presented in this chapter. For comparison to the constant property case, results with low heat transfer are used to verify codes by making comparisons with established constant property results. Then, results with significant heat transfer are considered. Buoyancy effects were included in all cases. Two different grid sizes, \((48\times48\times24)\) and \((48\times48\times48)\), were used. All cases employed in a \(2\pi\delta\times2\delta\times\pi\delta\) computational domain in the \(x\) (streamwise), \(y\) (normal), and \(z\) (spanwise) directions, respectively, where \(\delta\) is the channel half width.

In this study, the Grashof number \((Gr)\) was based on the temperature difference between the two walls and the channel width, and is defined as

\[
Gr = \frac{g\beta(T_h - T_l)(2\delta)^3}{\nu^2}
\]  

(4.1)

where \(g\) is the gravitational acceleration, \(\beta\) is volumetric expansion coefficient, \(\delta\) is the channel half width, and \(\nu\) is the kinematic viscosity. The two temperatures and the channel width were considered as key variables in this study.

Two different wall temperature ratios \((\frac{T_h}{T_c})\) were investigated in order to establish both a low and high heat transfer rate. The low heat transfer rate employed a wall temperature ratio of 1.01 and the high heat transfer used a ratio of 3.0. To extend the investigation on the high heat transfer case, which is expected to make the properties vary significantly, use of both the wall friction velocity of the boundary walls and semi-local scaling will be compared as suggested in Huang et al. (1995). The detailed formulation is to be discussed later.

Besides the two temperature ratios, the inlet Mach number \((Ma)\) was varied from 0.009 to
0.070 in order to vary the buoyancy forces while keeping the Reynolds number nearly the same. The relationship between the Mach number (Ma) and the channel half width (δ) is given in the equations below.

\[ \delta = \frac{\nu Re}{u_{ref}} \]  

(4.2)

Since \( u_{ref} \) is defined as

\[ u_{ref} = Ma\sqrt{\gamma RT} \]  

(4.3)

Equation 4.2 becomes

\[ \delta = \frac{\nu Re}{Ma\sqrt{\gamma RT}} \]  

(4.4)

where \( \nu \) is the molecular kinematic viscosity, \( \gamma \) is the ratio of specific heats, \( R \) is the gas constant, \( T \) is the temperature, and \( Re \) is the Reynolds number.

Throughout this study, a Prandtl number (Pr) of 0.71 and the ideal gas law were used.

4.1 Large Eddy Simulation of Turbulent Channel Flow with Low Heat Transfer

4.1.1 Problem Description

In this section, the low temperature ratio was adopted to simulate the constant property case. The temperature ratio was kept small so that viscosity and density variations would not be significant. As a result, the results from this study can be compared to incompressible DNS (Kim et al., 1987) and experimental (Niederschulte et al., 1990) data. The purpose was to verify the computer code before executing high heat transfer rate cases. The dimensionless time step was \( 3.0 \times 10^{-2} \) and statistics were collected for 16,000 to 20,000 steps to reach a statistically stationary state flows. However, the number of steps required to reach a stationary state depended somewhat on temperature ratio and Mach number. The simulations were performed
using a Silicon Graphics Origin 200 workstation (180MHz CPU, MIPS R10000 processor chip) located at the Iowa State University Virtual Reality Application Center.

Simulations were carried out with both a central difference and an upwind scheme. Table 4.1 summarizes the flow parameters for the current simulations. The subscript $h$, and $c$ denote hot and cold walls, respectively. The Reynolds number based on the friction velocity $Re_{\tau} = \left( u_{\tau} \frac{\delta}{\nu} \right)$ varied between 170 and 180 because the density and viscosity are functions of wall temperature. Note that $Re_{\tau_c}$ is slightly higher because of the higher density near the cold wall side.

The dimensionless bulk velocity ($U_m$), bulk temperature ($T_m$), bulk density ($\rho_m$), and bulk Reynolds number ($Re_m$) are defined as follows.

\begin{equation}
U_m = \frac{\int_{-1}^{1} \rho u dy}{\int_{-1}^{1} \rho dy} \tag{4.5}
\end{equation}

\begin{equation}
T_m = \frac{\int_{-1}^{1} \rho u T dy}{\int_{-1}^{1} \rho u dy} \tag{4.6}
\end{equation}

\begin{equation}
\rho_m = \frac{\int_{-1}^{1} \rho dy}{\int_{-1}^{1} dy} \tag{4.7}
\end{equation}

and

\begin{equation}
Re_m = U_m \frac{\delta}{\nu_b} \tag{4.8}
\end{equation}

where $\nu_b$ is the bulk kinematic viscosity. Although its variation was small, the density variations were included in all the bulk calculations. In addition, Dean’s (1978) formulation based on experimental data for the ratio of the centerline and bulk velocities, $\frac{U_c}{U_m} = 1.282 Re_m^{-0.0116}$, for the constant property case is shown in the 6th column of Table 4.1. The simulated velocity ratios deviate by 3.0 and 8.0 percent from the Dean’s experimental correlation for the central and upwind schemes, respectively. The velocity profile should be symmetric for constant properties because the momentum and energy equations are decoupled. But when the compressible equations with heat transfer are employed, the profile may be non-symmetric.
Therefore, the maximum velocity does not generally occur at the centerline of channel. If the maximum values are used for the centerline velocity, then the deviations become 1.0 and 4.0 percent for the central and upwind schemes, respectively.

The bulk Richardson number $Ri_b = Gr/(Re_b)^2$ remains small because of the low temperature ratio. This allows the results to be compared to the previous incompressible DNS performed by Kim et al., 1987. The simulations listed in Table 4.1 were both carried out on 48x48x48 grids.

<table>
<thead>
<tr>
<th>CASE</th>
<th>$(T_h/T_c)$</th>
<th>$Re_\tau$</th>
<th>$Re_m$</th>
<th>$U_c/U_b$</th>
<th>Dean's</th>
<th>$Gr$</th>
<th>$Gr/Re^2$</th>
<th>Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.02</td>
<td>169 - 173</td>
<td>2718.72</td>
<td>1.15</td>
<td>1.16</td>
<td>19351.75</td>
<td>0.003</td>
<td>Central</td>
</tr>
<tr>
<td>2</td>
<td>1.02</td>
<td>175 - 184</td>
<td>3195.64</td>
<td>1.14</td>
<td>1.16</td>
<td>19351.75</td>
<td>0.002</td>
<td>Upwind</td>
</tr>
</tbody>
</table>

### 4.1.2 Analysis

#### 4.1.2.1 Mean properties

The mean velocity profile scaled by the friction velocity is defined as

$$< u^+ > = \frac{< u >}{u_\tau} \quad (4.9)$$

where the friction velocity is

$$u_\tau = \sqrt{\frac{\tau}{\rho}}_{wall} \quad (4.10)$$

and

$$y^+ = \frac{y u_\tau}{\nu_{wall}} \quad (4.11)$$

The collection of statistics is based on the following equation.

$$\bar{u}_i = < u_i > + \bar{u}_i'' \quad (4.12)$$
Equation 4.12 shows that the averaging is performed in time and the homogeneous directions (x and z). Figure 4.1 compares the mean velocity profiles of cases 1 (central difference) and 2 (upwind). Both plots show good symmetry about the channel centerline. This indicates that the time averaging for the mean velocity reaches a steady state. The same velocity profiles, but normalized by the wall friction velocity, are plotted in wall coordinates in Fig. 4.2. case I shows excellent agreement with the DNS data of Kim et al. (1987), the experimental data of Niederschulte et al. (1990), and LES data of Dailey et al. (1998) along with the empirical correlations of the linear viscous sublayer \( u^+ = y^+ \), with \( u^+ = u/\overline{u}_r \) and the logarithmic law of the wall \( u^+ = (1/k)\log y^+ + 5.5 \) with \( k = 0.40 \).

Figure 4.2 shows the mean temperature and density profiles. Both temperature and density were scaled by their reference values \( (T_0 \text{ and } \rho_0) \). These plots also show symmetry about the channel centerline. The two temperature profiles agree well. The density profiles, as expected,
are almost unity because of the low $T_{top}/T_{bottom}$ ratio of 1.01 which was used.

Figure 4.4 shows the mean temperature profiles in wall coordinates. The temperature is scaled as $<\theta^+> = (T - T_{wall})/T_\tau$ where the friction temperature is $T_\tau = q_{wall}/\rho_{wall}C_p u_\tau$. The reference LES data are from Dailey et al., 1998 performed for a channel flow with an isoflux wall boundary condition. Again, the empirical correlations of the linear viscous sublayer ($\theta^+ = Pr y^+$) and the logarithmic law of the wall ($\theta^+ = 2.78\ln y^+ + 2.09$) are given on the figure. Both the central and upwind schemes show good agreement with the reference data. It is noted that the linear relation near the central region is related to the inflexion point.

### 4.1.2.2 Turbulence Intensities

The $rms$ values of the two components of the resolved velocity fluctuations, $<u'^2>^{1/2}$, and $<v'^2>^{1/2}$ are shown in Figs. 4.5 and 4.6. The data are compared to DNS (Kim et al., 1987), and experimental (Niederschulte et al., 1990) data. Case 1 agrees well in the near wall region for both the $u_{rms}$ and $v_{rms}$ plots. Since the temperatures of the top and bottom walls are only slightly different from the reference temperature, the fluctuations closely resemble the passive
Figure 4.3 The mean temperature and density profiles in global coordinates. See Fig. 4.1 for further caption. Central and upwind represent case 1 and case 2.

Figure 4.4 The mean temperature profiles in global coordinates. See Fig. 4.1 for further caption. Central and upwind represent case 1 and case 2.
Figure 4.5  $u_{rms}$ plot. Central and upwind represent case 1 and case 2

Figure 4.6  $u_{rms}$ plot. Central and upwind represent case 1 and case 2
scalar case. Case 2, again, over-predicted the fluctuation of the $u$ velocity plot, however $v_{rms}$ shows reasonably good agreement with the incompressible data.

The $uv$ velocity cross-correlation coefficient, $R(uv)$, was calculated by

$$\begin{align*}
R(uv) &= \frac{<u'v'>}{u_{rms}v_{rms}} \\
&= (4.13)
\end{align*}$$

Figure 4.7 shows the cross-correlation coefficient and very good agreement is noted for both cases 1 and 2.

Figures 4.8 - 4.11 show the time-averaged velocity vector plots in streamwise direction. At the beginning of the simulation, the flow is not smooth and is somewhat chaotic. However, as time goes on, the velocity profiles become smooth, indicating that the flow reaches a fully-developed state.

Another time-averaged plot is shown in Fig. 4.12. This temperature plot shows that there is no temperature gradient in the streamwise direction. Since an isothermal wall boundary condition was imposed, the temperature gradient existed in the normal direction only.

![Figure 4.7 Velocity cross-correlation coefficient. Central and upwind represent case 1 and case 2](image-url)
Figure 4.8  Initial streamwise velocity vector plot in the channel with low heat transfer

Figure 4.9  After 180 dimensionless time steps

4.1.2.3 Instantaneous Plots

Figures 4.13 and 4.14 show the instantaneous velocity and temperature plots in the y-z plane. Note that there are significant motions near the wall. However, no significant motions are found in the middle region.

4.2 Large Eddy Simulation of Unstably Stratified Turbulent Channel Flow

LES of the fully developed horizontal channel flow under unstably stratified flow conditions (see Fig. 4.15) was carried out to investigate the effect of the buoyant force on the momentum and heat transport. To investigate this, Gr has been changed from 2,820 to 1,327,280 by changing the initial velocity field. All other conditions, including boundary temperature ratio, geometry, and reference primitive variables were identical for both cases. The buoyant force is known to play a role in the transport mechanism of near wall turbulence and in the central

Figure 4.10  After 300 dimensionless time steps
region.

4.2.1 Problem Description

When the density or thermal stratification is unstable dynamically, large-scale thermal convection occurs and this phenomenon changes the transport mechanism of the near wall region (Lumley et al., 1978). According to Kasagi et al., 1997, the diffusion transports kinetic energy between near the wall and the central region under unstably stratified flow.

In this section, two cases having significantly different Grashof numbers are discussed. Both cases were considered unstably stratified fully-developed channel flow. Due to limited resources, a coarse grid (48x48x24) was used with initial Reynolds number, $Re = 3200$, based on the initial center line velocity and channel half width. The detailed description of these two cases is given in Table 4.2.
Figure 4.13 Instantaneous vector plot in y-z plane

Figure 4.14 Instantaneous temperature plot in y-z plane

Table 4.2 Parameters for low and high Gr cases with high heat transfer

<table>
<thead>
<tr>
<th>CASE</th>
<th>( \frac{T_h}{T_c} )</th>
<th>( Re_m )</th>
<th>( Gr )</th>
<th>( Gr/Re^2 )</th>
<th>Scheme</th>
<th>Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>3.0</td>
<td>2802.75</td>
<td>2820.96</td>
<td>0.0004</td>
<td>Upwind</td>
<td>48x18x24</td>
</tr>
<tr>
<td>4</td>
<td>3.0</td>
<td>3218.81</td>
<td>1327280.12</td>
<td>0.1312</td>
<td>Upwind</td>
<td>48x48x24</td>
</tr>
</tbody>
</table>
The bulk Richardson number \(\left(= \frac{Gr}{Re^2}\right)\) is an indicator of the importance of buoyancy and is different for the two cases. For comparison purposes, the same scheme and grid size were used throughout this study. There have been two parameters analyzed for heat and momentum transports, and they are the Nusselt number and skin friction coefficient defined by

\[
Nu = \frac{4h\delta}{k_b} \quad (4.14)
\]

\[
C_f = \frac{2\tau_w}{\rho_b U_b^2} \quad (4.15)
\]

where \(h\) is the heat transfer coefficient, \(\delta\) is the channel half-height, \(k_b\) is the bulk thermal conductivity, \(\tau_w\) is the wall shear stress, \(\rho_b\) is the bulk density, and \(U_b\) is the bulk streamwise velocity. Due to the high temperature ratio and instability of flow, the total number of time steps have been significantly increased compared to the low heat transfer case. Both cases 3 and 4 simulations were terminated after 35,000 time steps (dimensionless step size 0.01). The simulation was performed using a Silicon Graphics Inc. Origin 2000 parallel computer (300 MHz CPU, MIPS R12000 processor chip) located at Iowa State University Computational Center.

Figure 4.15 The configuration of unstably stratified channel flow
4.2.2 Analysis

Figure 4.16 shows the mean velocity distribution normalized by the wall friction velocity. Because of the large density and viscosity variations for the high temperature ratio case, the profiles are broken into two parts, one associated with each wall. It is not very easy to investigate the effect of buoyancy with this velocity plot. Therefore, a semi-local scaling has been utilized as suggested in Huang et al. (1995), and it is shown in Figs. 4.17 and 4.18 for the cold and hot walls, respectively. Figure 4.17 shows that cases 3 and 4 agree well in the sub-layer region, but they diverge toward the central region of the channel. Unlike Fig. 4.17, Fig. 4.18 indicates both cases 3 and 4 are nearly identical. The mean velocity distribution normalized by the bulk mean velocity in global coordinates is shown in Fig. 4.19. It should be noted that they are markedly different at the center of the channel. With the buoyancy effect, the central part of the velocity profile has been leveled off where the large flux Richardson number occurs (Wang, 1995).

Figure 4.20 shows the temperature distribution scaled by the wall friction temperature. Like Fig. 4.16, the viscosity and density have a large effect on the profiles. However, it is clear that the large Gr affects the temperature distribution significantly. Temperature profiles in global coordinate can be observed in Fig. 4.21. In the central region of the channel, the profile of the high Grashof number case has been flattened indicating the high buoyancy effect. This is due to the tight coupling between the velocity and temperature for high heat transfer with variable properties. This figure also illustrates the buoyancy effects on the heat transfer near the wall. As can be seen, the temperature gradients of the high Grashof number case are much higher near the hot and cold walls. In other words, the effects of buoyancy are very effective in transporting heat near the wall.

Figure 4.22 shows the changes in the Nusselt number, and skin friction coefficient, normalized by the reference Nusselt number, and skin friction coefficient computed at \( \text{Gr} = 2820.96 \), versus the Grashof number. When Grashof number increases, the normalized Nusselt number increases, as well. Again, the buoyancy effects are proven to be very effective in transporting heat, as discussed earlier. Unlike the Nusselt number, the skin friction coefficient ratio
Figure 4.16  Law of the wall plot scaled by the wall friction velocity

Figure 4.17  Law of the wall with semi-local scaling, cooled side.
Figure 4.18  Law of the wall with semi-local scaling, heated side.

Figure 4.19  Mean velocity scaled by bulk velocity in global coordinates.
Figure 4.20 Temperature distribution scaled by the wall friction temperature in wall coordinates.

Figure 4.21 Original temperature profile in global coordinates. Since cold and hot dimensionless temperature are set as 0.5 and 1.5 ($\frac{T_h}{T_c} = 3.0$), the range of the temperature is from 0.5 to 1.5.
decreased to 0.157 when the Grashof number increased to 967587.72. Then, as the Grashof number continued to increase, the skin friction coefficient ratio increased to 4.68. This is because the turbulence has been enhanced as Grashof number increase.

As shown in Fig. 4.23, the decrease of the mean velocity distribution is mainly due to the increase of $-u^+v^+$ in the near wall region. This considerable increase of $-u^+v^+$ is generally thought to be related to the increase of buoyancy (Kasagi et al., 1997).

The turbulence intensities($rms$) are shown in Figs. 4.24 and 4.25 for primitive velocities,
Figure 4.24 $u_{rms}^{+}$ plot in global coordinates. $u_{rms}$ near hot (heated) and cold (cooled) walls.

Figure 4.25 $v_{rms}^{+}$ plot in global coordinates. $v_{rms}$ near hot (heated) and cold (cooled) walls.
u and v for the cooled and heated walls. As can be seen, the values vary drastically in the near wall region for both $u_{\text{rms}}^{+}$ and $v_{\text{rms}}^{+}$ plots. The values of $u_{\text{rms}}^{+}$ for the profiles near the heated side increase and the difference reaches a maximum near the wall, then decreases towards the central region. In contrast, the effect of Grashof number on $u_{\text{rms}}^{+}$ is smaller near the cooled wall. However, the difference increases toward the central region of the channel. The distribution of $v_{\text{rms}}^{+}$ shows a similar trend, but the difference in the intensities markedly increases in the outer region. This significant difference in the velocity fluctuations illustrates the two different Gr effects on the turbulence intensities.

The time-averaged fully-developed velocity vector plot is shown in Fig. 4.26 for case 3 (low Grashof number). The velocity vector profile looks very similar to that of the low heat transfer case (Fig. 4.11). In other words, the vector profiles aren't noticeably affected by temperature difference or heat transfer rate.

Figures 4.27 and 4.28 show the instantaneous turbulent velocity vector, and temperature plots in the y-z plane for a low Grashof number (case 3). Note that no significantly large scale motions are detected across the channel. In other words, eddies do not extract energy strongly from the mean flow, and no significant turbulent motions can be sustained to transfer heat in the channel central region.

The time-averaged fully-developed velocity vectors are shown in Fig. 4.26 for case 4 (high Grashof number). As mentioned above, the velocity vector profile looks very similar to the low heat transfer case (Fig. 4.11).

The instantaneous turbulent velocity and temperature for case 4 (high Grashof number) are plotted in Figs. 4.30, and 4.31 in the y-z plane. It is clearly seen that more vigorous motions are observed across the channel than for the low Grashof number case (case 3). The thermal convection emerged from near the wall pushes the low-speed fluid to the central region. Strong vortices which normally carry large amounts of energy are observed in the near-wall region.
Figure 4.26  Time averaged fully-developed streamwise velocity vector plot in streamwise direction for case 3 (low Grashof)

Figure 4.27  Instantaneous turbulent velocity vector plot in y-z plane for case 3 (low Grashof)
Figure 4.28  Instantaneous temperature plot in y-z plane for case 3 (low Grashof)

Figure 4.29  Time averaged fully-developed streamwise velocity vector plot for case 4 (high Grashof)
Figure 4.30  Instantaneous turbulent velocity plot in y-z plane for case 4 (high Grashof)

Figure 4.31  Instantaneous temperature plot in y-z plane for case 4 (high Grashof)
4.2.3 Characteristics of Variable Properties

Due to the significant temperature difference between the top and bottom boundary walls, the effects of variable viscosity and conductivity are expected to be significant, too. In this subsection, the influence of variable properties is to be analyzed to determine if mean velocity, Reynolds stress, \( r_{\text{rms}} \) turbulent velocity profiles are asymmetric. Since the introduction of a variable property is the only concern, the low Grashof number case (case 3) was used.

Figure 4.32 shows the mean velocity scaled by the initial centerline velocity. The flow has its maximum value offset from the centerline and the profile is non-symmetric. The maximum value is 0.9322 at \( y = -0.0325 \). It is noted that the maximum value has shifted toward the cold wall which has a lower viscosity. This profile tells the fact that the velocity profile is not affected much by density changes.

Figure 4.33 shows the resolved Reynolds shear stress across the channel. Like the velocity profile, it is asymmetric and again, the absolute maximum value has moved toward the cold wall. The maximum value near the cold wall is 0.5450 at \( y = -0.8072 \) and 0.5296 at \( y = 0.692 \) near the hot wall.

The \( r_{\text{rms}} \) velocity profiles are shown in Fig. 4.34. The minimum values correspond to the maximum value of the mean velocity profile. Unlike the above two profiles, the higher value of \( u_{\text{rms}} \) is found near the hot wall. However, the peak values of the other two profiles, \( v_{\text{rms}} \) and \( w_{\text{rms}} \), occur close to the cold wall. All three profiles are non-symmetric.

4.3 Large Eddy Simulation of Unstably and Stably Stratified Turbulent Channel Flows

In many engineering applications, two types of convections, forced and natural, appear together. This is referred to as a stratified flow if the mean flow is driven horizontally. Depending on the direction of heat transfer, the stratified flow is identified as either stable or unstable (see Figs. 4.35 and 4.36).

It is known that when unstable stratification is imposed, turbulence is enhanced, but turbulence is diminished and eventually relaminarized under strongly stable stratification.
Figure 4.32 Mean velocity scaled by initial centerline velocity, case 3 in global coordinates.

Figure 4.33 Resolved shear stress plot for case 3 in global coordinates.
(Narashimha and Sreenivasam, 1979; Kasagi and Iida, 1997).

In this research, both stably and unstably stratified flow have been studied extensively and the complexity of the buoyancy and the heat transfer was investigated. The quantitative and qualitative studies were executed in the near wall and central regions to determine the turbulent structures at these locations. Also, instantaneous plots are used to show the intensified or depressed ejection associated with the thermal plumes and the vortices in the near wall region.

4.3.1 Problem Description

Two different cases of buoyancy effects, stable and unstable, were considered with the same temperature ratio \( T_h/T_b = 3.0 \), and the same grid size \( (48^3) \) using the upwind scheme. The configurations for this study are shown in Figs. 4.35, and 4.36. As a result of the isothermal boundary condition at the top and bottom walls, and neglecting the effects of the pressure variations on density, a fully developed state for both the velocity and temperature variables can be achieved.

Due to the unstable nature of unstably stratified flow, a dimensionless time step of \( 1.0 \times 10^{-2} \) was used which is three times smaller than for the low heat transfer case. For stably stratified flow, \( 2.0 \times 10^{-2} \) was used for the time step. The development to the fully developed state was much slower compared to the low heat transfer case and required about 20,000 to 25,000 steps.
It is believed that the slow development of the turbulent thermal field is due to the coupling of the temperature and velocity. The computation was performed using the Silicon Graphics IRIX 6.5.5f operating system on the Origin 2000 (195MHz CPU, MIPS R10000) located at the University of Illinois at Urbana-Champaign.

### 4.3.2 Analysis

Table 4.3 shows the details of the cases. The definitions of $Re_T$, $Re_m$, and Grashof number remain same as in section 4.1.1. As one can observe, the $Re_T$ near the hot wall is much smaller than near the cold wall as a result of the density and viscosity variation effects. This large difference of $Re_T$ alters the turbulent structures near the wall.

The turbulent kinetic energy (TKE) was obtained by the use of temporally and spatially averaged turbulent velocities as

$$TKE = \frac{1}{2} \left< u_i \right> \left< u_i \right>$$  \hspace{1cm} (4.16)
where \( \overline{\omega_i} \) is the vector of the three dimensionless velocity components.

Figure 4.37 shows the turbulent kinetic energy in wall coordinates. As can be seen, the turbulent kinetic energy for both the stable and unstable cases is intensified near the cold wall, whilst the turbulent kinetic energy decreases near the hot wall. The alternation of \( Re_x \) (or viscosity) changes the size of the turbulent structures. The large turbulent structures appear near the hot wall (Nicoud, 1999).

Table 4.3 Comparison of stable and unstable stratification for high heat transfer rate using upwind scheme

<table>
<thead>
<tr>
<th>CASE</th>
<th>( \frac{T_h}{T_c} )</th>
<th>( Re_m - Re_x )</th>
<th>( Re_m )</th>
<th>( Gr )</th>
<th>( Gr/Re^2 )</th>
<th>Scheme</th>
<th>Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>3.0</td>
<td>80 - 380</td>
<td>2769.77</td>
<td>967587.71</td>
<td>0.13</td>
<td>Upwind</td>
<td>48x48x48</td>
</tr>
<tr>
<td>6</td>
<td>3.0</td>
<td>80 - 380</td>
<td>2769.77</td>
<td>967587.71</td>
<td>0.13</td>
<td>Upwind</td>
<td>48x48x48</td>
</tr>
</tbody>
</table>

Figure 4.38 shows the mean velocity distribution in the streamwise direction scaled by average of the wall friction velocities. The profiles are non-symmetric and are influenced by the different viscosities near the walls. The steep velocity gradients are observed indicating the presence of a viscous sub-layer. It is clear that the unstable buoyant force in the central region of the channel results in a flattened mean velocity profile. It appears that the unstably stratified flow enhances the turbulence and the stably stratified flow suppresses the turbulence.

![Figure 4.37 Turbulent kinetic energy. Note that case 5 is stable case and case 6 is unstable case](image-url)
Since the ideal gas law was used in the present study and the pressure was almost constant across channel, the mean density was inversely proportional to the temperature. This effect can be observed in Fig. 4.39. Since both the stably and unstably buoyant force cases imposed a large temperature difference at the boundary walls, the mass flow rate, \((=\rho u)\), was considerably larger near the cold wall than near the hot wall. This large variation was mainly due to the significant density change.

Figure 4.40 shows the mean velocity normalized by the wall friction velocity in semi-logarithmic coordinates. Since the friction velocity was not the same value on both walls, the local friction velocities at the top and bottom walls were utilized in the plots. As can be seen, the profile for the top and bottom walls are different from the passive scalar DNS result (Kim et al., 1987), and experimental data (Niederschulte et al., 1990) due to the fact that the density and viscosity vary significantly. Some researchers (Simpson et al., 1988) used the mean friction velocity to minimize this difference, but using the mean friction velocity is contradictory to the concept of "wall" coordinates.

Instead of using the mean friction velocity, a semi-local scaling as suggested in Huang et al. (1995) appealed more to the author. \(u_\tau^*\) and \(y^*\) are defined by \(u_\tau^*(y) = \sqrt{\frac{\tau_w}{\rho(y)}}\), and \(y^* = \frac{y u_\tau^*}{v(y)}\). This semi-local scaling reflects the local variables well compared to the wall coordinates. These plots are shown in Figs. 4.41, and 4.42 for the cold wall, and hot wall, respectively.
Comparison with the results obtained by Dailey et al. (1998), Kim et al. (1987), Niederschulte et al. (1990) and the correlation of the law of the wall are shown.

As observed in section 4.2.2, the mean velocity distribution and the Reynolds shear stress are closely related. Under unstable stratification, the mean velocity in the channel central region tends to decrease and this is mainly due to the increase of the shear stress. Figure 4.43 indicates the same trend observed in section 4.2.2. The shear stress of the unstable stratification increases and this higher stress causes the decrease of the mean velocity as shown in Figs. 4.41, and 4.42.

The turbulent intensities near the wall are shown in Figs. 4.44, and 4.45. The velocity components, u, v, and w scaled by the wall friction velocity are plotted in global coordinates. It is apparent that the buoyancy forces affect the turbulent intensities significantly. Generally, the unstable configuration enhances the intensities near the wall and the channel central region.

Figure 4.47 shows the mean temperature across the channel. As discussed in Tennekes and Lumley, 1972, the buoyancy generated eddies are quite effective in transporting heat. It can be observed in Fig. 4.47 that the larger temperature gradient, especially near the hot wall, for
Figure 4.40  The mean velocity scaled by wall friction velocity in wall coordinates

Figure 4.41  Mean velocity plot near cooled wall side in semi-local scaling
the unstable buoyancy case is indicating higher heat transport.

The different heat transport for cases 5 and 6 can be described quantitatively by means of the Nusselt number. Table 4.4 shows the Nusselt number scaled by the reference Nusselt number (=29.8) taken at $Gr = 2820.96$. It shows that the heat transport for the stable buoyancy case is lower than the unstable buoyancy case as discussed above.

The instantaneous turbulent velocity and temperature plots are shown in Figs. 4.48 - 4.51. It is not clear to the author how the stable and unstable buoyant forces affected the turbulent structures. For stable stratification, relatively large scale motions are observed near the cold wall, and no significant motion is found at the center line. Under unstable stratification, more large scales and significant velocity movements are found.

<table>
<thead>
<tr>
<th>CASE</th>
<th>$(Nu/Nu_0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.95</td>
</tr>
<tr>
<td>6</td>
<td>1.08</td>
</tr>
</tbody>
</table>
Figure 4.43  Reynolds shear stress plot near the hot wall

Figure 4.44  \( u_{rms} \) plot near the hot wall
Figure 4.45 $u_{rms}$ plot near the hot wall

Figure 4.46 $w_{rms}$ plot near the hot wall
Figure 4.47 Original mean temperature plot. Since cold and hot dimensionless temperature are set as 0.5 and 1.5, the range of the temperature is from 0.5 to 1.5 as shown in y axis.
Figure 4.48 The instantaneous turbulent velocity vector plot for stable stratification

Figure 4.49 The instantaneous temperature plot for stable stratification
Figure 4.50  The instantaneous turbulent velocity vector plot for unstable stratification
Figure 4.51  The instantaneous temperature contour plot for unstable stratification
5 CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Large eddy simulations of fully developed horizontal isothermal wall channel flow under stable and unstable buoyancy conditions were carried out with heat transfer at a Reynolds number \( \text{Re} = 3200 \) based on the initial centerline velocity and the channel half width. Low Mach number preconditioning was employed to avoid inefficiencies at low Mach number. Two different spatial discretizations were used, central and upwind on a staggered grid, and the results of simulations were studied using statistical analysis of the unsteady data.

For validation purposes, a low heat transfer case was simulated using the central and upwind schemes. Since the temperatures of the boundary walls, scaled by the reference temperature, were almost unity, the results were compared to the passive scalar DNS performed by Kim et al., 1987, and experiment data of Niederschulte et al., 1990, and reasonably good agreement was noted.

The mean velocity profiles scaled by the wall friction velocity showed that the upwind scheme over-predicted, but not significantly, in the central region of the channel compared to the results of the central difference scheme which showed a good agreement with the incompressible DNS data. Similar trends were observed for the mean temperature. No significant differences between the results of the central and upwind schemes were observed in other profiles such as the mean velocity scaled by the bulk velocity, the mean temperature scaled by the initial reference temperature, the density scaled by the initial reference density, and the velocity cross-correlation coefficient in global coordinates.

LES of the fully developed horizontal turbulent channel flow under unstable buoyancy forces has been carried out to investigate the effects of buoyancy on the turbulent structures.
for two different Grashof numbers. With increasing Grashof number, large scale turbulent motions emerged near the wall and those motions extracted the energy from the mean velocity resulting in flattened mean velocity and temperature distributions.

Increasing the Grashof number affected the temperature profiles because of the coupling between velocity and temperature. The dimensionless root-mean-square velocity fluctuations were drastically changed near the hot wall. However, no significant change was observed near the cold wall. This result indicated that the turbulent structures were influenced by buoyancy near the hot wall even if the buoyant production was relatively small in that region.

The instantaneous turbulent velocity plots also showed the effects of buoyancy. The thermal convection emerging from the wall region convects low-speed fluid to the central region. The high-speed fluid was also forced to move near the boundary wall by this convection.

Finally, a comparison of LES of unstably and stably stratified turbulent channel flow has been performed. The results were compared to DNS and experimental data, and the buoyancy effects of the two different cases were discussed.

For the unstably stratified flow case (or unstable buoyancy case) the resolved Reynolds shear stress was observed to increase somewhat with Grashof number. This increase of the shear stress was associated with the decrease of the mean velocity near the central region of the channel. The turbulent intensities were also affected by the buoyancy. Generally, an unstable buoyant force enhanced the intensities whilst a stable buoyant force suppressed the intensities near the wall.

This study showed that LES with property variation can be very useful for analyzing the buoyancy effects on the turbulent structures, momentum and heat transport for the high heat transfer case. This study also provided information on buoyancy effects with significant property-variations which is more likely to exist in engineering application.

### 5.2 Recommendation for Future Research

Despite the efforts and accomplishments achieved in this study, there is much that should be resolved before LES is used as an important engineering tool.
The central difference discretization scheme should be applied to the high heat transfer case. This should improve the accuracy as it did for the low heat transfer case in this study. However, the computational stability problem should be resolved for strong buoyancy before the central difference scheme is used.

As for the simulations involving heat transfer, it would be interesting to include both buoyancy effects and rotation which should lead to an increase in turbulence levels if the system rotation acts to destabilize the flow. As discussed by Piomelli et al., 1995, the destabilizing effects of rotation on turbulence in channel flow would be quite challenging since the SGS model should capture inactive turbulence motions as well as fully-developed turbulence. An improved dynamic subgrid-scale stress model is needed in order to remove the mathematical inconsistency to any order of accuracy in time.
APPENDIX A  APPROXIMATION OF SURFACE AND VOLUME INTEGRALS

1. Approximation of Surface Integrals

As a beginning, the finite volume method uses the integral form of the conservation equation and the domain is subdivided by a finite number of control volumes(CV). Depending on two dimensional or three dimensional CVs, the CV surface can be subdivided into four or six faces.

Generally, the net flux can be expressed as

\[ \int_S f dS = \sum_k \int_{S_k} f dS \]  \hspace{1cm} (A.1)

where \( f \) is either the convective or diffusive vector. To compute the surface integral, an approximation should be adopted. The simplest one is the midpoint rule which was used in this study. This method is defined as

\[ F = \int_{S_k} f dS \approx f_k S_k \]  \hspace{1cm} (A.2)

where subscript \( k \) denotes the face and \( S \) is the magnitude of area.

Another approximation is the trapezoidal rule, which defined as

\[ F = \int_{S_k} f dS \approx \frac{S_k}{2} (f_{nk} + f_{sk}) \]  \hspace{1cm} (A.3)

where subscripts \( nk \) and \( sk \) denote the north and south corner of face, respectively.

So far, both the midpoint and trapezoidal rules are of second order. For higher order, more than two locations need to be known. Simpson’s rule, which is of fourth-order, can approximate the surface integral as follows;
\[ F = \int_{S_k} f dS \simeq \frac{S_k}{6} (f_{nk} + 4f_e + f_{sk}) \]  
(A.4)

Here, three locations are used; two corners and a center of face.

2. Approximation of Volume Integrals

In representing a conservation statement by the finite volume method, there were two volume integrals that needed to be approximated. The simplest second-order accurate approximation and the one used in this study utilized the mean value theorem. It is given by

\[ V = \int_v UdV \simeq U_p \Delta V \]  
(A.5)

where P is the point at the CV center.

Since all the values at P are known, interpolation is not necessary, but due to nonlinear variation in the control volume, the above equation has a second-order error.

To increase the order of accuracy, more points need to be known, and these points are found by interpolation. For instance, if one wants to use a fourth-order approximation in a two-dimensional CV, the function U can be represented as

\[ U = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2 + a_5 xy + a_6 x^2 y + a_7 xy^2 + a_8 x^2 y^2 \]  
(A.6)

Then, the integration gives

\[ V = \int_v UdV \simeq \Delta x \Delta y [a_0 + \frac{a_3}{12} (\Delta x)^2 + \frac{a_4}{12} (\Delta y)^2 + \frac{a_8}{144} (\Delta x)^2 (\Delta y)^2] \]  
(A.7)

Only four coefficients need to be determined by fitting the function to the values of U.

By use of same method, extending to a three-dimensional CV should be straightforward.
APPENDIX B  WALL BOUNDARY CONDITIONS

The implementation of boundary conditions on the staggered grid requires the concept of a "ghost" or fictitious cell as it is shown in Fig B.1.

This fictitious point, noted as g, was used to compute all the primitive values at that point. To find the relation with other neighboring points, a three-point polynomial extrapolation has been used in this study. The derivation of the equation is as follows:

The general equation is \( f = a + by + cy^2 \). If the given condition is applied

\[
T_1 = a + b(\Delta y_1) + c(\Delta y_1^2)
\]

\[
T_2 = a + b(\Delta y_1 + \Delta y_2) + c(\Delta y_1 + \Delta y_2)^2
\]

\[
T_3 = a + b(\Delta y_1 + \Delta y_2 + \Delta y_3) + c(\Delta y_1 + \Delta y_2 + \Delta y_3)^2
\]

Since there are three unknowns (a, b, and c) and three equations, a, b, and c can be determined.

Figure B.1 The configuration near the boundary wall.
BIBLIOGRAPHY


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