Università degli Studi di Trieste

XXVI Ciclo del Dottorato di ricerca in Environmental and Industrial Fluid Mechanics

Wall-layer modelling of massive separation in Large Eddy Simulation of coastal flows

Settore scientifico-disciplinare: ICAR/01

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Academic Year 2013–2014
Acknowledgement

I would like to thank all the people who supported, helped and encouraged me to write this Ph.D thesis.

- **Professor Vincenzo Armenio**, my kind supervisor, without his help, support and advice it was not possible to accomplish this dissertation. Having a chance to work under his guidance was an honor for me to experience research influenced by his wide academic knowledge.

- **Dr. Federico Roman** who gently guided me well, and kept me in the right direction of doing this project step by step.

- **Dr. Andrea Petronio** and other colleagues who provided such a calm and friendly environment, made me so enthusiast to work in the Hydraulic Laboratory.

- All the professors and personnels of school of Doctorate in Environmental and Industrial Fluid Mechanics. Also the University of Trieste for the financial support and all the facilities.

- The University of Hawaii for their collaboration regarding the oceanic modelling of Kaneohe bay.

- The University of Malta for providing Albert supercomputer to run our simulations.

And **My mother** for all moral and material supports, and her patience.

*Thank you*
Abstract

The subject of modelling flow near wall is still open in turbulent wall bounded flows, since there is no wall layer model which works perfectly. Most of the present models work well in attached flows, specially for very simple geometries like plane channel flows. Weakness of the models appears in complex geometries, and many of them do not capture flow separation accurately in detached flows, specially when the slope of wall changes gradually.

In many engineering applications, we deal with complex geometries. A possible way to simulate flows influenced by complex geometry using a structured grid, is to consider the geometry as immersed boundary for the simulation. Current wall layer models for the immersed boundaries are more complex and less accurate than the body-fitted cases (cases without immersed boundaries).

In this project the accuracy of wall layer model in high Reynolds number flows is targeted, using LES for attached flows as well as detached flows (flows with separation). In addition to the body fitted cases, wall layer model in the presence of immersed boundaries which is treated totally different also regarded. A single solver is used (LES – COAST\(^1\)) for the flow simulations, and the aim is to improve wall layer model in the cases with uniform coarse grid.

This is in fact novelty of the thesis to introduce a wall layer model applied on the first off-wall computational node of a uniform coarse grid, and merely use LES on the whole domain. This work for the immersed boundaries is in continuation of the methodology proposed by Roman et al. [30] in which velocities at the cells next to immersed boundaries are reconstructed analytically from law of the wall.

In body-fitted cases, since smaller Smagorinsky constant is required close to the walls than the other points, wall layer model in dynamic Smagorinsky sub-grid scale model using dynamic \(k\) (instead of Von Karman constant) is applied to optimize wall function in separated flows. In the presence of immersed boundaries, the present wall layer model is calibrated, and then improved in attached and also detached flows with

\(^{1}\)IE-Fluids, University of Trieste.
two different approaches. The results are also compared to experiment and resolved LES. Consequently the optimized wall layer models show an acceptable accuracy, and are more reliable.

In the last part of this thesis, LES is applied to model the wave and wind driven sea water circulation in Kaneohe bay, which is a bay with a massive coral reef. This is the first time that LES – COAST is applied on a reef-lagoon system which is very challenging since the bathymetry changes very steeply. For example the water depth differs from less than 1 meter over the reef to more than 10 meters in vicinity of the reef, in lagoon. Since a static grid is implemented, the effect of wave is imposed as the velocity of current over the reef, which is used on the boundary of our computational domain. Two eddies Smagorinsky SGS model is used for this simulation.
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Chapter 1

Introduction

In many engineering applications, it is too costly or even impossible to make an experimental set-up or to use analytical approaches for the analysis of a fluid flow. Availability of high performance computers in the recent years has made it possible to use numerical algorithms to analyse fluid flows. Computational fluid dynamics (CFD) is a tool to compute quantities of interest of the fluid such as velocity, pressure, density, temperature.

The flow in which transport of momentum is mainly governed by diffusive transport due to molecular viscosity action is called laminar. Quantities have a fixed value after reaching a steady state condition in this kind of flow. Computation of the fluid quantities in laminar flow is the simplest simulation in CFD, which can be easily performed by Direct Numerical Simulation (DNS).

In nature we often deal with turbulent flows, in which the different layers of fluid flow mix with each other due to advective transport, and molecular viscosity becomes unimportant. The behaviour of the flow is chaotic, dissipative, with strong mixing, including large amount of vorticity, variables randomly in time and space, and so there is not an exact solution for it.

Turbulent flows contain a variety of time- and length-scales. DNS resolves all the scales, but for very high Reynolds numbers it is not feasible to be used even on a simple geometry. In order to model a turbulent flow with DNS, a resolution of $Re^3$ for a three dimensional simulation is required, where $Re = ul/ν$ is Reynolds number which is a function of a characteristic inertial velocity $u$, length scale $l$, and kinematic viscosity $ν$. In turbulent flows, different time- and length-scales exist. Larger eddies continuously break down to smaller eddies so that very small eddies dissipate energy to heat due to viscosity. Therefore it is reasonable to resolve larger scales and model smaller scales.

Large Eddy Simulation (LES) is based on the aforementioned principle. In LES,
large and energy carrying eddies which depend on the geometry, are directly computed explicitly. Smaller scales, which are more isotropic, transmit energy to the smaller scales (energy cascade) which finally dissipate energy; the small scales, not resolved in LES are modelled, using a sub-grid scale (SGS) model. The main purpose of SGS models is to represent energy transfer in a statistical sense.

Wall bounded flows, specially at high Reynolds numbers, need a high resolution near the wall to be simulated, because of the need to solve the thin viscous sub-layer. In LES, this resolution is comparable with the one needed in Direct Numerical Simulation (DNS). As far as Reynolds number increases the cost of a wall-resolving LES increases with $Re^{2.5}$. Also for applications where wall roughness is the rule rather than the exception, it does not make sense to describe in a deterministic sense the wall boundary.

The most practical way of simulating a wall-bounded, high Reynolds number flow, is to consider coarse grid, and model the nodes next to the wall with a wall function. This function is supposed to mimic the presence of solid wall in the near-wall flow. Several wall models have been introduced. All of them have weaknesses, and work well in certain conditions. This subject is still challenging for improvement.

The aim of this research project is to develop a wall layer model in attached flows as well as detached flows, to have capability of predicting separation with an acceptable accuracy. The preference is to have a uniform coarse grid and use LES for all the domain, near wall as well as farther. The single solver applied for the simulations in this project is LES – COAST which is used to model coastal flows. Standard and dynamic Smagorinsky models are used as SGS models. In chapter 2 problem formulation and sub-grid scales model applied in LES – COAST are explained.

A body-fitted (also called boundary fitted) case is the case in which a structured curvilinear grid is generated to follow the geometry. In this case, a certain length scale can be defined based on the grid size for all the domain. Since the grid border overlapping edge of the geometry, all quantities are defined in a universal frame of reference, and boundary conditions are imposed on the certain grid nodes. This facilitates to compute all the vectors and also gradients in Navier-Stokes equations. Meanwhile all cells of the domain capture the fluid flow.

In complex geometries where the structured grid can not follow it, another approach is applied to deal with the geometry as immersed boundary (solid wall). The grid domain can be Cartesian or curvilinear. In this way a length scale can not be defined for near wall points since they do not depend on the domain any more, therefore another approach than Navier-Stokes must be applied to compute velocities in near wall points. For this issue, a local frame of reference must be introduced to identify normal and
tangential directions to the immersed boundary at each near wall node. Hence the quantities are calculated first in local frame of reference and then are transformed to the universal frame of reference. In this case specially when a Cartesian grid is applied, some cells can not capture the fluid flow and so called wasted.

Chapter 3 reviews different kinds of wall layer models which have been developed to be used for LES in body-fitted cases and also using immersed boundaries. The wall function for body-fitted cases (in the absence of immersed boundaries) is equilibrium stress model, based on law of the wall. Details of wall layer models available in LES – COAST are explained in chapter 4.

In chapter 5 of this thesis, the wall layer model is applied in the cases which there is flow separation. Different resolutions are tested, and the results are compared with experiments for validation. After that, we use a single uniform coarse grid for all the domain, and develop a wall layer model for separated flows. We test the model in the case of a plane channel flow and obtain an inflow for another case which is flow over a single hill in body-fitted case.

Implementation and optimization of the immersed boundary methodology are illustrated in chapter 6. First the current immersed boundary method developed by Roman et al. [30] is tested and calibrated in order to conserve momentum in our simulation. Then optimization is carried out in plane channel flow which is a standard attached boundary layer. Finally in this chapter a detached flow is discussed and a theory is derived from boundary layer equations to optimize the immersed boundary methodology in separated flow. This new theory is applied on a single hill, and then is also tested on periodic hills; in these problems the prediction of the separation and re-attachment points constitute a challenging task.

Finally in chapter 7, the model is applied to the study of a coral reef bay (Kaneohe bay, Oahu, Hawaii) a very challenging site from a modelization point of view, due to the discontinuous bathymetry associated to the contemporary presence of sand banks and reef formations. To the best of our knowledge:

- this is the first time where a high-definition LES model is applied to the analysis of mixing and turbulent transport in the Kaneohe bay. In fact, Lowe et al. [22] applied a 3D coupled wave circulation model to the complex coral reef system in Kaneohe bay, using Delft3D to couple currents iteratively with wave transformations simulated by the numerical wave model SWAN,

- this is the first time where the model LES – COAST is used in such a challenging case. Petronio et al. [24] applied LES model for wind driven sea circulation in
Muggia bay. Galea et al. [14] studied mixing and water renewal in the Barcelona harbour using LES – COAST. In both studies, the authors used wind forcing over the free surface by the formula proposed by Wu [44] in which the induced stress at the surface of sea is calculated from the velocity of wind at 10 meter above the mean sea level. In this work in addition to the wind forcing, we also impose the effect of wave as current velocity over the reef considering the wave friction law proposed by Hearn [16].
Chapter 2

Problem formulation

Turbulent flows which are commonly observed in environment and also industrial processes, appear chaotic, unsteady, and irregular since they behave randomly. Velocity of the flow field changes tangibly in an unpredictable form in time and space, and this is the main feature of turbulent flows. Turbulent flows transport and mix fluid much more efficiently than laminar flows. Turbulence is inherently non linear implying energy transfer among different scales and vortex stretching and tilting in a flow, it is rotational and three dimensional.

The vortex stretching transfers energy and vorticity to smaller scales and so on, finally when the gradients are large, they dissipate mechanical energy into heat due to viscosity. Meanwhile turbulent flows are diffusive since there is a fast diffusion rate of momentum and heat by viscous shear stress due to high mixing. Turbulence is also identified by fluctuating vortex structures in different scales; these structures are called eddies, and they can be visualized in enormous scales in different forms such as stretching and spinning.

A turbulent flow includes eddies with many different length scales, and the range of scales is powerfully dependent on the Reynolds number. Figure 2.1 shows Large and small scales in mixing layer. Large scales containing the most part of kinetic energy of the flow while small scales transform energy to the smaller and smaller scales which is called energy cascade. Finally the smallest scale dissipates the energy to heat since the molecular viscosity becomes very important. The smallest scale in which dissipation occurs is called Kolmogorov length scale.

In DNS all the scales even the Kolmogorov scale must be resolved. The computational domain must be much larger than the large scales while the resolution of the grid must be so high to capture smallest scales. In addition to length scale, time advancement of simulation is also dependent on the Reynolds number and it must be very small.
for resolving the small scales. Wall bounded flows more severely depend on Reynolds number, because when Reynolds number increases the small fluid structures decrease in size rapidly. To avoid huge cost and in many cases impossibility of DNS specially in high Reynolds numbers, LES is a common model to resolve large scales and model small scales with a sub-grid scale (SGS) model.

2.1 LES – COAST model

This solver can be applied for LES modelling of either atmospheric or oceanic flows. Using curvilinear grid to follow the geometry and also capability of using immersed boundaries to create complex geometries have made LES – COAST (Roman et al. [32]) very useful for a variety of industrial and environmental applications. There are several SGS models available for smaller scale in the solver such as standard Smagorinsky, dynamic Smagorinsky and Lagrangian models.

In this chapter, the basis of LES – COAST solver which is used for the simulations is described. First the flow equations are presented, then filtering, SGS models (standard and dynamic Smagorinsky ones, which were used for this work); also the wall layer models implemented in this solver are described for both cases with presence and absence of the immersed boundaries.

2.1.1 Navier-Stokes equations

The governing equations for fluid motion are Navier-Stokes equations. In most of industrial and environmental applications, the fluid can be considered incompressible under Boussinesq approximation which means density variation is negligible in comparison with velocity gradient in continuity equation. In momentum equations also we can ignore these variations, but just in vertical direction these variations effect the motion through buoyancy term. This assumption could be correct under this condition that density deviation inside the fluid is only a fraction of the state of reference $\rho_0$. 
2.1. LES – COAST MODEL

Considering an incompressible flow, the continuity, momentum and energy equations in Cartesian coordinate are written below. In this project we do not consider heat transfer, so the energy equation is not used.

\[ \frac{\partial u_i}{\partial x_i} = 0, \quad (2.1) \]

\[ \frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{\rho}{\rho_0} g \delta_{i,2} + B_i , \quad (2.2) \]

\[ \frac{\partial T}{\partial t} + \frac{\partial u_j T}{\partial x_j} = k \frac{\partial^2 T}{\partial x_j \partial x_j} . \quad (2.3) \]

Index 1 is in stream-wise \((x)\) direction, 2 is in wall-normal \((y)\) direction, and 3 is in span-wise \((z)\) direction, so after this we use \(x\) referring to \(x_1\), \(y\) referring to \(x_2\), and \(z\) referring to \(x_3\). Also velocities \(u, v, w\) referring to \(u_1, u_2, u_3\) respectively. \(p\) is pressure, \(\nu\) the kinematic viscosity of the fluid, \(g\) the gravitational acceleration, \(\rho\) the density deviation from the reference density, \(\rho_0\) the bulk or reference density, and \(B\) the body force other that gravity, as, for example, Coriolis force \((2\Omega_i \times u_i)\) where \(\Omega_i\) is the angular velocity of Earth.

\[ \frac{\rho}{\rho_0} g \delta_{i,2} \] is a buoyancy term in which the effect of density variations in vertical direction can influence the fluid \((g \delta_{i,2} = (0, -g, 0))\), \(k\) is the coefficient of thermal diffusion. Density in the model is assumed to depend on just temperature as a linear function, so that

\[ \frac{\Delta \rho}{\rho_0} = -\alpha_T \Delta T , \]

where \(\alpha_T\) is the thermal expansion coefficient. Equation\((2.3)\) represents the advective-diffusion of temperature, in which \(k\) is the thermal diffusion coefficient. This equation is used generally for any scalar; such as temperature and salinity. In this project we have not considered scalar, therefore this equation is not used.

As mentioned before, large eddies are more influenced by the boundary conditions, whereas small eddies are more universal. Therefore it is reasonable to resolve the large scales more accurately and model the smaller scales as it is done in LES. To capture well the large eddies, we need a velocity field containing just the large scale components of the whole field. The scale separation is performed applying a filter to the turbulent variables. Assuming \(f\) as a turbulent variable, the filtered variables (resolved, or large scale), denoted by an overbar defined as below.

\[ \overline{f}_i(x) = \int_D f_i(x') dx' G(x, x'), \quad (2.4) \]

where \(D\) is the entire domain and \(G\) is the filter function. This divides the variables into two parts and gives: \(f_i = \overline{f}_i + f'_i\), in which \(\overline{f}_i\) is the part related to the large scale,
and \( f_i \) related to the SGS. The filter function we use in this solver is top-hat filter defined as
\[
G(x) = \begin{cases} 
\frac{1}{\Delta} & \text{if } |x| \geq \frac{\Delta}{2} \\
0 & \text{elsewhere.}
\end{cases}
\] (2.5)

The structures larger than \( \Delta \) are simulated and those smaller than the filter size are modeled with a SGS model. Filtering is applied to the equations of fluid motion, and substituting \( u_i = \bar{u}_i + u_{sgs,i} \) and \( p_i = \bar{p}_i + p_{sgs,i} \), the filtered Navier-Stokes equations for a Newtonian and incompressible flow assume the following form:
\[
\frac{\partial \bar{u}_i}{\partial x_j} = 0 ,
\] (2.6)
\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - 2\Omega_i \times \bar{u}_i - \frac{\bar{p}}{\rho_0} g \delta_{i,2} ,
\] (2.7)
\[
\frac{\partial T}{\partial t} + \frac{\partial (\bar{u}_i T)}{\partial x_j} = k \frac{\partial^2 T}{\partial x_j \partial x_j} - \frac{\partial \lambda_j}{\partial x_j} .
\] (2.8)

These filtered Navier-Stokes equations simulate the evolution of larger scales, while the effect of smaller scales appears as the SGS stress term \( \tau_{ij} \) in the momentum equation and as SGS heat flux \( \lambda_j \) in energy equation:
\[
\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j ,
\] (2.9)
\[
\lambda_j = \bar{u}_j T - \bar{u}_j T .
\] (2.10)

These terms must be modelled by a SGS model. Since in this project we do not deal with heat transfer, we just consider modelling of SGS stress term. There are different SGS models, and here we describe the models which are applied by LES – COAST solver.

### 2.1.2 Standard Smagorinsky model

SGS models used in our solver are based on eddy viscosity model, which relate small scales (SGS) stresses \( \tau_{ij} \) to the large scale strain tensor. Most of the eddy viscosity models are in the general form of:
\[
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_T \mathbf{S}_{ij} ,
\] (2.11)

where \( \mathbf{S}_{ij} \) called large scale strain rate tensor, and it is defined as:
\[
\mathbf{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) ,
\] (2.12)
\( \nu_T \) is SGS turbulent viscosity, also known as eddy viscosity. Substituting this term for SGS stresses \( \tau_{ij} \) in the filtered Navier-Stokes equations, we can write:

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + (\nu + \nu_T) \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j}. \tag{2.13}
\]

The first SGS model was introduced by Smagorinsky for LES of an urban atmospheric flow in 1963. This model is based on the equilibrium hypothesis; this assumption comes from considering that small scales have shorter time scale than large ones, and recover much faster to equilibrium in perturbations, almost instantaneously. Therefore all terms drop in SGS turbulent energy equation except the production \( \epsilon_{sgs} = \tau_{ij} \mathbf{S}_{ij} \) term and viscous dissipation \( \epsilon_v \); finally considering the length scale \( l \sim \bar{\Delta} \), the eddy viscosity can be written as below.

\[
\nu_T = (C_s \bar{\Delta})^2 |\mathbf{S}|, \tag{2.14}
\]

In which \( C_s \) is the constant of the model (the Smagorinsky constant), and \( |\mathbf{S}| = \sqrt{2 \mathbf{S}_{ij} \mathbf{S}_{ij}} \) is contraction of strain rate tensor of the large scale; \( \mathbf{S}_{ij} \). Finally, the SGS stresses are calculated as:

\[
\tau_{ij} = -2\nu_T \mathbf{S}_{ij}. \tag{2.15}
\]

The Smagorinsky constant is commonly considered between 0.065 and 0.2, the filter width is proportional to the grid size in all directions, and is equal to \( \bar{\Delta} = 2(\Delta x \Delta y \Delta z)^{1/3} \). A drawback appears near the walls, where the eddy viscosity is expected to vanish, but in this method it is large because of the large value of strain rate tensors. To overcome this problem, other methods have been introduced such as, among the others, the dynamic model, the mixed model, the scale similar model. Here the dynamic model used in this project is discussed.

### 2.1.3 Dynamic Smagorinsky model

In the dynamic model, the model coefficient is calculated at each cell, instead of setting a value which is used in standard Smagorinsky SGS model. This is carried out by defining an additional test filter (denoted by a caret), and its width \( \hat{\Delta} \) is larger than the grid filter width \( \bar{\Delta} \), here is \( \hat{\Delta} = 2\bar{\Delta} \). As it was mentioned before, effect of small scales appears in the sub-grid scale term (2.9), \( \tau_{ij} \) inside the momentum equation, which must be modelled. Applying the additional test filter on the momentum equations, we will have:

\[
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial (\tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} + \nu_T \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j}, \tag{2.16}
\]
where $T_{ij}$ called subtest stresses:

$$T_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j,$$

(2.17)

considering the resolved turbulent stresses $L_{ij}$ defined as

$$L_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j,$$

(2.18)

These stresses represent the contribution to the SGS stresses by intermediate length scales; i.e. the length scales smaller than the test filter width $\hat{\Delta}$ and larger than the grid filter width $\bar{\Delta}$. They can be written as an algebraic relation:

$$L_{ij} \equiv T_{ij} - \hat{\tau}_{ij},$$

(2.19)

Figure 2.2 shows subtest stresses, resolved and SGS scales. Considering the Smagorinsky SGS model, we can model anisotropic parts of $\tau_{ij}$

$$\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} \simeq -2C\bar{\Delta}^2 \hat{S} \hat{S}_{ij} = -2C\alpha_{ij},$$

(2.20)

Also model the anisotropic part of $T_{ij}$,

$$T_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} \simeq -2C\hat{\Delta}^2 \hat{\hat{S}} \hat{\hat{S}}_{ij} = -2C\beta_{ij},$$

(2.21)

In which

$$\hat{\hat{S}}_{ij} = \frac{1}{2} \left( \frac{\partial \hat{u}_i}{\partial x_j} + \frac{\partial \hat{u}_j}{\partial x_i} \right), \quad |\hat{\hat{S}}| = \sqrt{2 \hat{\hat{S}}_{mn} \hat{\hat{S}}_{mn}}.$$  

(2.22)

Substituting $\tau_{ij}$ and $T_{ij}$, finally the error can be minimized in least-square sense. The error can be written as

$$e_{ij} = L_{ij} - T_{ij} + \hat{\tau}_{ij} = L_{ij} + 2CM_{ij},$$

(2.23)
2.1. **LES – COAST MODEL**

In which \( M_{ij} = \beta_{ij} - \tilde{\alpha}_{ij} \). Least-square minimization gives

\[
\frac{\partial E^2}{\partial C} = \frac{\partial \langle e_{ij} e_{ij} \rangle}{\partial C} = 0. \tag{2.24}
\]

Here \( \langle \rangle \) indicates average in homogeneity direction, parallel to the wall. Knowing that \( \frac{\partial \langle e_{ij} e_{ij} \rangle}{\partial C} = 2 \langle e_{ij} \frac{\partial e_{ij}}{\partial C} \rangle = 0 \), and also \( \frac{\partial e_{ij}}{\partial C} = 2M_{ij} \), we can write:

\[
\langle (L_{ij} + 2CM_{ij})M_{ij} \rangle = 0, \tag{2.25}
\]

therefore the coefficient can be calculated as:

\[
C = -\frac{1}{2} \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}. \tag{2.26}
\]

This \( C \) is called the dynamic constant, and then eddy viscosity can be calculated as below.

\[
\nu_T = C \hat{\Delta}^2 |\hat{S}| \tag{2.27}
\]

This ensemble average is carried out to get rid of the sharp functions which make instability to calculate this constant. The advantage of dynamic model over the standard one is that the eddy viscosity vanishes near the walls and in laminar flows, so, the model allows to treat transitional and wall bounded flow without the need to use special treatments of the constant.

### 2.1.4 Curvilinear coordinate

The Navier-Stokes equations mentioned before were written in Cartesian coordinates. In complex geometries, curvilinear coordinates may have the advantage to follow the physical shape of the boundaries. The LES – COAST code is written in terrain following curvilinear coordinate system. In this section the strategy of transformation from Cartesian coordinates \((x_i)\) to curvilinear ones \((\xi_i)\) is described (see fig. 2.3). Atmospheric flows over hill and oceanic flow in bay are two examples of this kind. This makes an easy imposition of the boundary conditions on the geometrical contour.

Velocity gradient in the Cartesian coordinate can be written as:

\[
\frac{\partial u_i}{\partial x_j} = \frac{\partial u_i}{\partial \xi_k} \frac{\partial \xi_k}{\partial x_j}. \tag{2.28}
\]

Transforming equations (2.1), (2.2) into curvilinear coordinate system in strong conservation law gives:

\[
\frac{\partial U_m}{\partial \xi_m} = 0, \tag{2.29}
\]

\[
\frac{\partial J^{-1}u_i}{\partial t} + \frac{\partial F_{im}}{\partial \xi_m} = J^{-1}B_i, \tag{2.30}
\]
in which \( F_{im} \) is defined as

\[
F_{im} = U_m u_i + J^{-1} \frac{\partial \xi_m}{\partial x_i} p - \nu G^{mn} \frac{\partial u_i}{\partial \xi_n},
\]

(2.31)

also \( B_i \) including the gravitational term,

\[
J^{-1} = \det \left( \frac{\partial x_i}{\partial \xi_j} \right)
\]

is the inverse of Jacobian or the volume of the cell,

\( U_m = J^{-1} \frac{\partial \xi_m}{\partial x_j} u_j \) is the volume flux (contravariant velocity multiply by \( J^{-1} \)) normal to the surface of constant \( \xi_m \),

\( G^{mn} = J^{-1} \frac{\partial \xi_m}{\partial x_j} \frac{\partial \xi_n}{\partial x_j} \) is called mesh skewness tensor. Also the scalar equation can be written as below.

\[
\frac{\partial J^{-1} \rho}{\partial t} + \frac{\partial U_m \rho}{\partial \xi_m} = \frac{\partial}{\partial \xi_m} \left( kG^{mn} \frac{\partial \rho}{\partial \xi_n} \right).
\]

(2.32)

In the next section, discretization and the procedure to solve the discretized equations are described.

### 2.1.5 Discretization and computational procedure

The solution of equations (2.29) and (2.30) is based on fractional step method, described in Zang et al. [45]. Spatial discretization in the computational space \( \xi, \eta, \) and \( \zeta \), is carried out using second order central finite differences. In non-staggered grids pressure and Cartesian velocities are defined at the cell centre while contravariant fluxes are defined at the boundary of cells as shown in fig. 2.3. Contravariant fluxes are displayed with capital letters.

Temporal integration is carried out by using the second order accurate Adams – Bashforth scheme for the convective term, and implicit Crank – Nicolson scheme for the diagonal viscous terms. A collocated grid is considered where pressure and Cartesian
velocity components are defined at the cell center, and the volume fluxes are defined at the mid points of the cell faces. Discretizing the momentum equation gives:

\[
J^{-1} \frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} = \frac{3}{2} (C_{i}^{n} + D_{E}(u_{i}^{n}) + B_{i}^{n}) - \frac{1}{2} (C_{i}^{n-1} + D_{E}(u_{i}^{n-1}) + B_{i}^{n-1}) + R_{i}(p^{n+1}) + \frac{1}{2} (D_{I}(u_{i}^{n+1} + u_{i}^{n})) \tag{2.33}
\]

Here superscripts show the time step and \(C_{i}\) represents the convective terms. Also \(R_{i}\) is the gradient operator in curvilinear form (for the pressure gradient terms), \(D_{I}\) is the diagonal viscous term which treated implicitly and \(D_{E}\) represents the off-diagonal diffusive term treated explicitly.

\[
C_{i} = - \frac{\partial}{\partial \xi_{m}} (U_{m} u_{i}), \tag{2.34}
\]
\[
R_{i} = - \frac{\partial}{\partial \xi_{m}} \left( J^{-1} \frac{\partial \xi_{m}}{\partial x_{i}} \right), \tag{2.35}
\]
\[
D_{I} = \frac{\partial}{\partial \xi_{m}} \left( \nu G_{mn} \frac{\partial}{\partial \xi_{n}} \right), \quad m = n \tag{2.36}
\]
\[
D_{E} = \frac{\partial}{\partial \xi_{m}} \left( \nu G_{mn} \frac{\partial}{\partial \xi_{n}} \right), \quad m \neq n. \tag{2.37}
\]

Applying the fractional step method, and instead of calculating directly \(u_{i}^{n+1}\) in equation (2.30), an intermediate velocity \(u_{i}^{*}\) is used first to predict the time advancement of the advective and diffusive momentum transport. This step is called predictor:

\[
\left( I - \frac{\Delta t}{2J^{-1}} \right) (u_{i}^{*} - u_{i}^{n}) = \frac{\Delta t}{J^{-1}} \left[ \frac{3}{2} (C_{i}^{n} + D_{E}(u_{i}^{n}) + B_{i}^{n}) - \frac{1}{2} (C_{i}^{n-1} + D_{E}(u_{i}^{n-1}) + B_{i}^{n-1}) + R_{i}(p^{n+1}) + \frac{1}{2} (D_{I}(u_{i}^{n+1} + u_{i}^{n})) \right] \tag{2.38}
\]

in which \(I\) is the identity matrix. Now in the corrector step, velocity at the next time step is computed to enforce continuity through the pressure:

\[
u_{i}^{n+1} - u_{i}^{*} = \frac{\Delta t}{J^{-1}} [R_{i}(\phi^{n+1})] \tag{2.39}
\]

The projector operator \(\phi\) has a relation with the pressure as below.

\[
R_{i}(p) = \left( J^{-1} - \frac{\Delta t}{2} D_{I} \right) \left( \frac{R_{i}(\phi)}{J^{-1}} \right) \tag{2.40}
\]

A multi grid method considered to solve Poisson equation for the pressure field. The contravariant velocity is defined at the cell sides to avoid pressure oscillations. Also
a third order quadratic upwind interpolation scheme (QUICK) can alternatively be adopted for the spatial discretization of the convective terms. The Poisson equation is written as:

$$\frac{\partial}{\partial \xi_m} \left( G_{mn} \frac{\partial \phi^{n+1}}{\partial \xi_n} \right) = \frac{1}{\Delta t} \frac{\partial U^*_m}{\partial \xi_m}$$  \hspace{1cm} (2.41)

in which $U^*_m$ is the intermediate volume flux and is defined as:

$$U_m^{n+1} = J^{-1}(\partial \xi_m / \partial x_j) u_j^*.$$  

Finally the contravariant fluxes at the successive time instant are calculated.

$$U_m^{n+1} = U_m^n - \Delta t \left( G_{mn} \frac{\partial \phi^{n+1}}{\partial \xi_n} \right)$$ (2.42)

Filtering the continuity and momentum equations in curvilinear coordinate gives:

$$\frac{\partial U_m}{\partial \xi_m} = 0$$ (2.43)

$$\frac{\partial J^{-1} u_i}{\partial t} + \frac{\partial U_m u_i}{\partial \xi_m} =$$

$$- \frac{\partial}{\partial \xi_m} \left( \frac{\partial J^{-1} \xi_m}{\partial x_i} \right) - \frac{\partial}{\partial \xi_m} \frac{\partial \sigma_{mi}}{\partial x_i} + \frac{\partial}{\partial \xi_m} \left( \nu G_{mn} \frac{\partial u_i}{\partial \xi_n} \right) + J^{-1} B_i$$ (2.44)

The effect of smaller scales appears in $\sigma_{mi}$, which must be modelled.

$$\sigma_{mi} = J^{-1} \frac{\partial \xi_m}{\partial x_i} u_j u_i - J^{-1} \frac{\partial \xi_m}{\partial x_i} \frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial \xi_m} = \overline{U_m u_i} - U_m \overline{u_i}$$ (2.45)

This term is modelled using the contravariant counterpart of the SGS models described in sections 2.1.2 and 2.1.3 for Cartesian frame of reference. Finally, filtered scalar equation in curvilinear frame of reference is written as:

$$\frac{\partial J^{-1} C}{\partial t} + \frac{\partial U_m C}{\partial \xi_m} = \frac{\partial}{\partial \xi_m} \left( k G_{mn} \frac{\partial C}{\partial \xi_n} \right) - \frac{\partial \xi_m}{\partial x_j} \frac{\partial \lambda_i}{\partial \xi_m}$$ (2.46)

where $\lambda_i$ is the SGS density flux. The methodology described in this chapter is related to wall-layer resolved LES. In wall bounded high Reynolds number flows it is not economic or even possible to resolve very small eddies close to the wall. Next chapter is a literature survey on high Reynolds LES methods for skipping the resolution of the wall layer in body-fitted cases and also immersed boundaries.
Chapter 3

Literature survey on unresolved wall-layer LES

Resolving near wall region in wall bounded flows at high Reynolds numbers is not only a matter of cost, but it is also a matter of possibility. Considering a simple geometry like a plane channel flow, the cost for DNS is proportional to $Re^3$, and resolved LES is proportional to $Re^{2.4}$. Since the size of eddies near wall strongly depends on Reynolds number and their dimension reduces rapidly with an increase in Reynolds number, a very high resolution is required in this region. Hence wall resolved LES is limited to mild Reynolds numbers.

The most economical way doing LES in high Reynolds numbers and avoiding this huge cost is to consider coarse grid near wall and model the effect of wall layer region instead of resolving it. In recent years modelling near wall has been proposed by different wall functions. Since near wall resolution is low in this case, very sharp velocity gradients and eddies which transfer energy to outer region (the region farther from wall) can not be captured, the model must be able to express accurate wall shear stress to the outer region. In the next section the most common and important wall layer models are reviewed.

3.1 Equilibrium stress models

In this approach, the grid is generated in such a way that the first computational node (near the wall) is located in the log region. So, based on law of the wall, the horizontal velocity, either instantaneous or mean (a kind of temporal or spatial) can be fitted to determine wall stress. These models in which stress is obtained from logarithmic law of the wall, are called equilibrium-stress models and are valid only under the equilibrium
Assumption.

Applying LES on plane channel flow at large Reynolds numbers, Deardorff [10] and Schumann [34] assumed there is an equilibrium stress layer near wall, used the outer flow velocity to calculate wall stress based on logarithmic law. Therefore velocity can be written as below.

$$U^+_1 = \frac{1}{k} \log (y^+_1) + B, \quad (3.1)$$

in which $k$ is Von Karman constant, $U^+_1$ is non-dimensional plane averaged velocity at the near wall node, $y^+_1$ is the distance of this node from wall in wall units, and coefficient $B$ is between 5 and 5.5. At lower distance from the wall ($y^+_1 < 11$), this logarithmic law changes to linear law, i.e. $U^+_1 = y^+_1$. In this way the cost of the simulation is only related to the outer region which is in order of $Re^{0.5}$ [26]. Deardorff [10] limited the second order velocity derivative in vertical direction and imposed law of the wall in this way.

$$\frac{\partial^2 \bar{\pi}}{\partial y^2} = -\frac{1}{k y^+_1} + \frac{\partial^2 \bar{\pi}}{\partial z^2}, \quad (3.2)$$

$$\frac{\partial^2 \bar{w}}{\partial y^2} = \frac{\partial^2 \bar{w}}{\partial x^2}. \quad (3.3)$$

Where $\bar{u}$ and $\bar{w}$ are filtered stream-wise and span-wise velocities at the first computational node. Equation (3.2) forces mean velocity gradient to follow logarithmic law. Schumann [34] obtained the plane averaged wall shear stress $<\tau_w>$ from plane averaged velocity at the first grid point, using iterative method so that the shear velocity is computed from law of the wall from the averaged velocity.

$$\tau_{w,x}(x,z,t) = \frac{<\tau_w>}{U} \bar{u}(x,y_1,z,t), \quad (3.4)$$

$$\tau_{w,z}(x,z,t) = \frac{<\tau_w>}{U} \bar{w}(x,y_1,z,t), \quad (3.5)$$

where $\bar{u}(x,y_1,z,t)$ and $\bar{w}(x,y_1,z,t)$ are instantaneous filtered stream-wise and span-wise velocities at the first computational node, $<\tau_w>$ is plane averaged wall shear stress and $U$ plane averaged near wall velocity. Also Piomelli et al. [27] considered wall shear stress from instantaneous velocity in Schumann’s equations at some distance in stream-wise direction from the first point to describe better the elongated structures close to wall. In Overall, equilibrium stress models work well when turbulence is equilibrium. If it is not, they may fail, like in rotating channel.

These models are the least expensive wall layer models. They also provide roughness corrections easily from the logarithmic law modification, which is an important feature.
3.2. ZONAL APPROACH

Figure 3.1: Inner and outer grids in TLM, with courtesy of Piomelli and Balaras [26].

in environmental and oceanographic flows. By the way they are weak in cases with a marginal separation, or strong pressure gradient.

3.2 Zonal approach

In other approaches which are generally named as zonal models, stress derives from the solution of a separate set of equations on a finer mesh close to the wall, called two layer model (TLM); these models have problems in case a perturbation extends from the wall to the outer layer. This model proposed by Balaras and Benocci [2] who applied turbulent boundary layer equations on near wall region and LES on the outer layer. Boundary layer equations are written below.

\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial (\overline{u}_i \overline{u}_j)}{\partial x_j} = -\frac{\partial P_o}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ (\nu + \nu_t) \frac{\partial \overline{u}_i}{\partial x_j} \right], \quad i = 1, 3. \tag{3.6}
\]

\[
\overline{u}_2 = -\int_0^y \left( \frac{\partial \overline{u}_1}{\partial x_1} + \frac{\partial \overline{u}_3}{\partial x_3} \right) dy. \tag{3.7}
\]

Where \( \frac{\partial P_o}{\partial x_i} \) is the pressure gradient in outer region. In this model a finer grid is considered between the wall and first computational node of the coarser grid (see fig. 3.1). Balaras and Benocci [2] used an algebraic eddy viscosity to parametrize all scales near wall,

\[\nu_t = (ky)^2 D(y) |\overline{S}|, \tag{3.8}\]

in which \( k \) is Von Karman constant, \( y \) the wall distance, \( |\overline{S}| \) strain rate tensor magnitude, and \( D(y) \) is damping function which guarantees the correct behaviour of eddy viscosity at the wall,

\[D(y) = 1 - \exp[-(y^+/A^+)^3], \tag{3.9}\]
where $A^+ = 25$. In addition to plane channel flow, this method was tested on square ducts and also rotating channel, the cases in which equilibrium stress model was not valid or even failed, and this method showed a good accuracy to simulate these flows. Meanwhile Cabot [5] applied this approach to simulate flow over a backward facing step with only 10% fewer than the resolved LES of its previous work. He found that stream-wise pressure has an important effect in boundary layer of TLM. In this case mean velocity and skin friction coefficient were predicted well.

Wang [42] used TLM to study the air-foil trailing edge flow, resulting a very high skin friction even in the flow attached region. Then he modified equation 3.8 setting a dynamic constant to guarantee $\nu_t$ inside the boundary layer equates $\nu_T$ from outer region SGS at the interface between two layers. This reduced the inner layer eddy viscosity and improved the results.

Since TLM weakly couples the two different models on interface, this method has a drawback in flows in which perturbation propagates from near wall zone to the outer region.

### 3.3 Hybrid RANS/LES methods

In other approaches called as hybrid methods, a single grid is applied, but the turbulence models are different in inner and outer layers. Detached Eddy Simulation (DES) is a hybrid approach proposed by Balaras et al. [3] as a method to highly compute separated flows.

In this method they considered stretched grid close to wall to resolve the boundary layer. RANS is applied in the inner and LES in the outer region. DES works good in separated flow with large separation since detached eddies are too important in these cases.

Since there is not zonal interface between the inner and outer layers, the velocity is smooth everywhere. Some weaknesses of this method are logarithmic layer mismatch between the two solvers and high grid resolution dependency near wall. Resolved stress is much lower than the modelled stress even far from RANS/LES interface. The total shear stress in plane channel flow only depends on the distance from the wall, therefore decline in eddy viscosity farther the RANS/LES interface affects on the velocity profile and makes it to have high gradient at transition into LES region. This phenomena called DES buffer layer. Therefore an additional work must be done to improve this issue.

Keating and Piomelli [19] added stochastic force in the interface region, accelerated
3.4 WALL-LAYER MODELLING USING IMMERSED BOUNDARIES

resolved eddies generation, and obtained better result. Also Temmerman et al. [40] applied Hybrid RANS/LES method in a channel flow constricted by hill, in order to calculate eddy viscosity in RANS region which was equal to $C_\mu \frac{l}{l_{mod}}$, where $l_{mod}$ is length scale and $k_{mod}$ the modelled turbulent kinetic energy, they computed the constant ($C_\mu$) in such a way to equate RANS eddy viscosity to LES eddy viscosity on the interface. They were able to improve mean velocity profile doing this procedure.

Although Hybrid RANS/LES method is good in flows with instabilities such as adverse pressure gradient and concave curvature, but it is weak in attached flows, in general the flows with low level of instability, and a false merging region could appear in the interface of RANS and LES. Since the grid near wall must be resolved, it is the most expensive wall layer models.

In addition to the three main wall layer models explained, there are other models which are not mentioned here. Different wall layer models work well under some special conditions and they have limitations.

3.4 Wall-layer modelling using Immersed boundaries

Applying immersed boundaries solve the problem of geometry complexity in the cases in which structured curvilinear grid can not follow the geometry. In this case quantities at the nodes near wall can not be computed by LES since there is not a certain length scale in this region. In addition to the length scale, local frame of reference is needed since the tangential and normal directions to wall can vary from a point to another.

Immersed boundaries can be considered using local forcing functions on the vicinity of the boundary. Fadlun et al. [11] applied body forces to allow the imposition of the boundary conditions on a given surface not coinciding with the computational grid. After this work applying unresolved near-wall LES on complex geometries using immersed boundary started. There are not many published works available on immersed boundaries with wall-layer modelling. Here the recent works are described.

Tessicini et al. [41] applied wall layer model LES in the presence of immersed boundaries to simulate the flow past a 25 degree, asymmetric trailing edge of a model hydrofoil at a Reynolds number based on free stream velocity and the hydrofoil chord ($C$) equal to $Re_C = 2.15 \times 10^6$. They used Turbulent Boundary Layer equations for modelling the wall layer. Their result had a deviation at the second off-wall node which was considered as the outer boundary for the wall model. This discrepancy was sensitive to the distance of the second node from the wall, and was more where the distance was longer.
Roman et al. [31] used direct forcing, reconstructed the velocity at near wall computational nodes from an interpolation bases on law of the wall, and simulated flow in a S shape duct, unsteady flow around a cylinder and also Stokes flow around a sphere. In this case they used Taylor series to interpolate velocity. Later they applied a trilinear interpolation which is more robust than the Taylor series when the near wall node is in stencil for interpolation [30], and they obtained good results in plane channel flow.

Posa and Balaras [28] proposed a new model-based near-wall reconstruction to account for the lack of resolution and provide correct wall shear stress and hydrodynamic forces. They used a zonal approach; boundary layer equations with fine grid resolution on a sphere and cylinder (called this case Full Boundary Layer FBL) in wall-layer and LES in outer region.

Then they considered coarser grid and set one node inside the boundary layer, omitted the convective term in boundary layer equations based on this fact that if the first point off the wall is located inside the boundary layer neglecting this term does not provide significant errors. They assumed constant pressure gradient between the first and second nodes, and obtained tangential velocity as a second order function with respect to the distance of the node from immersed boundary. They also computed wall normal velocity by the difference between upstream (at the interface) and downstream (at the wall) flow rates, calling this method Reduced Diffusion Model (RDM).

In other attempt, they improved the accuracy in the outer part of the boundary layer by expressing the tangential velocity at the first off-wall node as a third order function of the distance from the wall (a polynomial), and obtained the additional constant from the velocity gradient and farther point, calling this strategy Hybrid Reconstruction Method (HRM). They compared these methods with a linear velocity reconstructions and observed improvement in predicting the wall shear stress.

This procedure depends on the position of the first two nodes since pressure gradient is considered constant between those. The first node must be inside the boundary layer and the second should not be far from the edge of the boundary layer to give more accurate results. The Reynolds number in cylinder case was at $Re = 300$ and in sphere was at $Re = 1000$.

Chen et al. [8] also proposed a wall layer model based on Turbulent Boundary Layer Equations at high Reynolds number, for implicit LES in presence of the immersed boundaries. First they tested it on a turbulent channel flow in the range of Reynolds numbers based on shear velocity from $Re_{\tau} = 395$ to $Re_{\tau} = 100,000$ with minimum 20 cells inside the inner region for lower and 40 cells for higher Reynolds numbers.

Then they simulated flow over a back-ward facing step at Reynolds number based on
In the next chapter wall layer models available in LES – COAST are explained for the body-fitted cases and also with immersed boundaries.
CHAPTER 3. LITERATURE SURVEY ON UNRESOLVED WALL-LAYER LES
Chapter 4

A review of unresolved wall-layer LES in LES – COAST

In this chapter the wall-layer modelling available in LES – COAST to avoid resolving near wall region is described. First the wall function for body-fitted cases is explained which was implemented by Stocca et al. [37]. Then immersed boundary methodology proposed by Roman et al. [30] is mentioned.

4.1 Wall-layer model for body-fitted cases

As it was mentioned before, at high Reynolds numbers there are very small-scale structures of fluid flow near the wall and the extension of the viscous sub-layer is so thin that it is impractical to resolve the near-wall flow, therefore it must be modelled. Also, when wall roughness is present, it is impossible to reconstruct in a deterministic way the solid boundary. Thus, to deal with these situations, LES is considered on a coarse grid, and a wall layer model is applied to mimic the solid walls. Different wall layer models have been developed, but it is still challenging to model near wall region with high accuracy.

Since stresses can not be computed accurately in coarse grids, most of the wall layer models in the recent years supply wall stress as a boundary condition. These models are generally called wall stress models. There are two different approaches of determination of the wall stress in these models.

The wall layer model which is used currently in LES – COAST, is an equilibrium wall stress model. Wall stress is obtained from an instantaneous matching of velocity at the first off-wall centroid with the log law to the computed velocity profile. The non-dimensional distance of the near wall computational node is considered to check
whether it is in the log region. The law of the wall is imposed on the instantaneous horizontal velocity.

\[
  u_p^+ = \begin{cases} 
    \frac{1}{k} \ln(y_p^+) + B & \text{if } y_p^+ > 11 \\
    y_p^+ & \text{if } y_p^+ \leq 11
  \end{cases}
\]  

(4.1)

where \( u_p^+ \) is the instantaneous non dimensional velocity modulus at the first off-wall computational node \( P \), which has a distance \( y_p \) from the wall:

\[
  u_p^+ = \frac{u_p}{u_\tau} = \sqrt{\frac{u^2 + w^2}{u_\tau^2}}
\]

\( k = 0.41 \) is the Von Karman constant and \( B = 5.1 \). The friction velocity \( u_\tau \) is calculated from the velocity \( u_p \) at each \( P \) point and depends on the distance from the wall \( y_p^+ \), either from linear or logarithmic law of (4.1). Then wall shear stress \( \tau_w \) is calculated from friction velocity, i.e. \( \tau_w = \rho u_\tau^2 \).

Considering that the instantaneous surface stress has angles \( \alpha \) and \( \beta \) with respect to the stream-wise and span-wise directions respectively, the wall shear stress \( \tau_w \) which is obtained from (4.1), can be written as two components in \( x \) and \( z \):

\[
  \tau_{wx} = \tau_w \cos \alpha
\]

(4.2)

\[
  \tau_{wz} = \tau_w \cos \beta
\]

(4.3)

Assuming \( \alpha \) to be equal to the angle of deviation from \( x \) direction of the first off-the-wall velocity vector, it can be calculated as \( \alpha = \arctan(w_p/u_p) \). With this procedure, we do not require to know the tangential velocity at the wall. Since integral scale of the flow is larger than the grid size considered for LES, Smagorinsky model may not be suited for reproduction of the eddy viscosity value close to the wall.

In addition to this, a knowledge of the contraction of resolved strain rate tensor is required in order to use a SGS eddy viscosity at the wall in Smagorinsky model. Since the tangential velocity is not determined in this case, we do not know this quantity. Specially, when the grid is coarse near the wall, non zero velocity gradient terms which are expecting to lead \( \overline{S}_{ij} \) terms, become increasingly wrong since they are derived assuming no-slip condition.

Therefore we modify the leading terms of the strain rate tensor \( \overline{S}_{ij} \) based on the location of \( y_p \). If the first point \( P \) is in the logarithmic region the leading terms of strain rate tensor are set analytically as:

\[
  \overline{S}_{12} = \frac{u_x}{k y_p u_p} u
\]

(4.4)

\[
  \overline{S}_{32} = \frac{u_x}{k y_p u_p} w
\]

(4.5)
4.2. IMMERSED BOUNDARY METHODOLOGY

And if the $P$ is located in viscous layer, we have the linear velocity profile and

$$S_{12} = \frac{u_p^2}{\nu} \frac{u}{u_p}, \quad (4.6)$$

$$S_{32} = \frac{u_p^2}{\nu} \frac{w}{u_p}. \quad (4.7)$$

Consequently the value of eddy viscosity near the wall adjusts consistently with the imposed stress. However the wall layer model mentioned above is for smooth surfaces. If we deal with a rough surface with the roughness height $y_0$ (which is not the averaged roughness, but the extrapolated one from the measured shifted velocity profile) the velocity profile is:

$$u_p^+ = \frac{1}{k} \ln \left( \frac{y_p}{y_0} \right) \quad y_p > y_0 \quad (4.8)$$

Only simplified cases with a constant roughness height $y_0$ will be considered. The same procedure based on equations (4.4) to (4.7) can be done to modify the leading terms of $S_{ij}$.

This wall layer model is very economic, and accurate in attached flows. Its drawback is in separated flows as it will be discussed in chapter 5 in details. The logarithmic law does not capture separation, therefore in detached flows a stretched grid near wall is required to have more resolution and the near wall computational nodes must be inside the viscous layer.

In most of the engineering applications, we deal with complex geometry in which we have to use either boundary fitted unstructured mesh or multi domain curvilinear structured grids. Curvilinear structured grids are suitable to be used for a low or medium level of complexity; in very complex geometry a multi domain approach is required, which is not economic. Unstructured grids also require much more computational nodes than the structured meshes, and usually they must be moved or deformed depending on the velocity of the flow field.

### 4.2 Immersed boundary methodology

In this section, the technique which is used to tackle simulation of the flow over obstacles like buildings, etc. is described. This method is based on identification of solid regions in the computational domain, which are separated by means of an interface $\psi$. The solver LES – COAST uses direct forcing IB, developed by Fadlun et al. [11]. Applying the direct forcing approach, a forcing term is added on right hand side of the momentum equation and a mass source/sink term is added on the RHS of the continuity equation.
CHAPTER 4. A REVIEW OF WMLES IN LES – COAST

Figure 4.1: Ray-tracing method to identify fluid and solid nodes, in a) two dimensions, and in b) three dimensions, by Roman et al. [31].

to represent the solid bodies. The governing equations can be written as:

$$\frac{\partial U_m}{\partial \xi_m} = J^{-1}y,$$

(4.9)

$$J^{-1} \frac{\partial u_i}{\partial t} + \frac{\partial U_m u_i}{\partial \xi_m} =$$

$$- J^{-1} \frac{\partial p}{\partial \xi_m} \frac{\partial \xi_m}{\partial x_i} + \frac{\partial}{\partial \xi_m} \left( \nu G_{mn} \frac{\partial u_i}{\partial \xi_n} \right) + J^{-1} B_i + J^{-1} f_i .$$

(4.10)

The forcing term $f_i$ is the only important term which is added to account for the presence of immersed boundaries. This forces the velocities in the first off-the-wall fluid nodes (referred as IB node) which surrounds the interface $\psi$, to assume $u_{IB,i}$ compatible with proper boundary condition on $\psi$. IB nodes do not usually lie on the surface $\psi$, therefore a proper interpolation must be made among the surrounding nodes. The forcing term also depends on the velocities in these nodes.

Using Immersed Boundary Method, the solid and fluid regions must be specified in the computational domain before running the simulation. First, the $\psi$ surface is created as a bounded close body, and discretized in space using unstructured mesh of plane triangular elements, since they suit themselves better to the complex shape surfaces and the normal direction to these surfaces can be recognized unambiguously. Then the meshed $\psi$ surface is interfaced using a simple and robust ray-tracing procedure (described in Roman et al. [31]), in order to identify fluid and solid nodes.

The ray starts from one grid node and passes through the centroid of one arbitrary triangle element of the surface $\psi$, and the ray crosses $\psi$ a finite number of times. If it crosses the surface $\psi$ an odd number of times, the node is recognized as fluid and if it crosses an even number of times, it is considered as solid node (see fig 4.1) and this procedure is repeated for all grid cells. After recognition of solid and fluid nodes, the
4.2. IMMERSED BOUNDARY METHODOLOGY

Figure 4.2: Discretization of a fluid-solid interface with the presence of immersed boundary method by Roman et al. [30]. Solid square, empty square and empty circle represent solid, fluid and IB nodes respectively.

following types of points are also specified:

IB are the closest fluid nodes to $\psi$, i.e. the first fluid nodes off the immersed boundary. IP points are the intersection points between the immersed surface and the normal line passing through the IB nodes. PP nodes are placed as close as possible to the first fluid nodes where the governing equations are solved. Figure 4.2 shows the position of the nodes mentioned above. Velocity at PP point is interpolated from velocities at its surrounding points (empty square points in fig. 4.2). Then shear velocity at PP point is computed. When the distance of the IB nodes from wall in wall unit satisfy ($d_{IB}^+ = \frac{d_{IB} u_r}{\nu} > 11$, where $u_r$ is the shear velocity calculated from $u_{pp}$, the logarithmic law is assumed to hold both for IB and PP points, and based on law of the wall we can write:

$$U_{IB}^+ = \frac{1}{k} \log(d_{IB}^+) + B ,$$

and $$U_{PP}^+ = \frac{1}{k} \log(d_{PP}^+) + B ,$$

in which $k$ is the Von Karmann constant, and $B$ is also constant. These constant values are considered 0.41 and 5.1 respectively in the code. Subtracting $U_{PP}^+$ from $U_{IB}^+$, it gives

$$U_{IB}^+ = U_{PP}^+ - \frac{1}{k} \sqrt{\frac{\tau_w}{\rho}} \log\left(\frac{d_{PP}}{d_{IB}}\right).$$

(4.11)

This relation holds for the instantaneous velocity. If the non-dimensional distance of IB node from immersed boundaries is $d_{IB}^+ < 11$, velocity at the IB is obtained linearly. As in the viscous layer in which we have $U_{IB}^+ = d_{IB}^+$, concluding:

$$U_{IB} = \frac{d_{IB} u_r^2}{\nu}.$$  

(4.12)

The tangential velocity is obtained from (4.12) or (4.11), depending on $d_{IB}^+$. To obtain the wall normal velocity at IB node, a parabolic interpolation is carried out. Considering $U_n$ (index n referring to wall normal direction) as a parabolic function in the
general form we have $u_n = ay^2 + by + c$. Imposing three conditions to interpolate wall normal velocity at $IB$ node, in which velocity is known at $PP$ point, impenetrability holds at $IP$ node, and also normal velocity at the immersed boundary surface is equal to zero. Finally we have the wall normal velocity at $IB$ nodes interpolated in this way:

$$U_{n,IB} = U_{n,PP} \frac{d^2_{IB}}{d^2_{PP}}.$$  \hspace{1cm} (4.13)

Setting the velocity components at $IB$ nodes only is not enough to obtain accurate results. Also, since the integral scale of the first grid point is smaller than the others, SGS models can not be accurate enough. A reconstruction of shear stress at the cell face is done using a RANS-like eddy viscosity. Eddy viscosity at the $IB$ nodes are calculated analytically from mixing length theory from the equation

$$\nu_t = C_w ku_{_r} d_{IB},$$ \hspace{1cm} (4.14)

where $k$ is the Von Karman constant, and $C_w$ is an intensification coefficient to be determined such that the Reynolds shear stress is a fraction of the wall shear stress near the wall (where $\nu_T$ is set), and also the eddy viscosity must be imposed at the cell face. Consequently this coefficient can be written as:

$$C_w = \frac{\nu_t}{\nu_{t,an}} = \frac{\tau_F d_F}{\tau_w d_{IB}},$$ \hspace{1cm} (4.15)

where the index $F$ denotes a quantity calculated at the cell face, $d_F$ is the distance between cell face and immersed surface, $\nu_t = \frac{\tau_F}{\rho u_{_r}}kd_F$, and $\nu_{t,an} = \frac{\tau_w}{\rho u_{_r}}kd_{IB}$. A more detailed description can be found in Roman et al. [30].

This wall layer model is very economic since the velocity is just interpolated from the projection point $PP$, and works well in attached flows using very coarse grid. Since the interpolation is based on logarithmic law, and the velocity direction at the $IB$ node following the velocity at $PP$ node, this method has a drawback in separated flows even setting the $IB$ node inside the viscous layer. The discussion related to this issue will be carried out in chapter 6.
Chapter 5

Numerical Implementation and optimization for body-fitted cases

In this chapter, the wall layer model in LES – COAST which was explained in chapter 2 section 4.1, is tested on a detached flow; the simulation of flow over a hill is carried out in which there is flow separation. The accuracy of wall layer model is checked and then some optimizations are done to increase the preciseness of the wall function.

5.1 Flow over a hill

Since most of the wall layer models have weakness in capturing the start and end points of flow separation in detached flows, specially when the slope of the solid wall changes gradually, we work on flow simulation over a single hill which is a very challenging problem for wall layer models.

5.1.1 Geometry description

The geometry and boundary conditions collected from ERCOFTAC classic database, environmental flows area, case 69, and the wind tunnel experiment has been done by Khurshudyan et al. [20]. In this case the hill height is $H = 0.117\ m$, and the aspect ratio $a = 3H$, where $a$ is the amplitude of the hill. The hill geometry is shown in fig. 5.1.

The line equation of the hill is given parametrically by:
Figure 5.1: Hill geometry in which $H$ is the hill height, $a$ is the aspect ratio, with courtesy of ERCOFTAC, Environmental Flows.

\[
\begin{align*}
  x &= \frac{1}{2} \xi [1 + \frac{a^2}{\xi^2 + m^2(a^2 - \xi^2)}] \\
  y &= \frac{1}{2} m \sqrt{a^2 - \xi^2} \left[1 + \frac{a^2}{\xi^2 + m^2(a^2 - \xi^2)}\right]
\end{align*}
\]

in which $m = n + \sqrt{n^2 + 1}$ and $n = \frac{H}{a}$ is average slope. A domain is considered with stream-wise length: $x = -3$ to 2.34 m ($L_x = 5.34$ m), height: $y = 0$ to 1 m ($h = 1$ m), and the width (in span-wise direction): $z = 0$ to 1 m ($L_z = 1$ m).

The boundary conditions are given as below:

- Inlet condition: velocity given by a logarithmic law profile on rough surface:

\[
U = \begin{cases} 
  \frac{u_\tau}{k} \ln \left( \frac{y}{y_0} \right), & \text{if } y \leq h \\
  U_{ref}, & \text{if } y > h
\end{cases}
\]

$V = 0$

$W = 0$

in which $U$, $V$, $W$ are stream-wise, wall-normal and span-wise velocities respectively, $y$ is the height from the ground, $y_0 = 1.57 \times 10^{-4}$ m is the roughness characteristic height, $k = 0.41$ is the Von Karman constant, $u_\tau = 0.178$ m/s is the friction velocity, $U_{ref} = 4$ m/s is the free stream velocity, and $h = 1$ m is the boundary layer depth. Reynolds number based on shear velocity is $Re_\tau = u_\tau h / \nu = 1187$, where $\nu$ is the kinematic viscosity.

- Outlet condition: open boundary,

- Upper boundary: free slip,
5.1. FLOW OVER A HILL

- Span-wise condition: periodic.

Before simulating flow over the hill, an open channel considered, with the same cross-sectional size and resolution as the hill domain, with 7.12 m length (in $x$), 1 m height (in $y$), and 1 m width (in $z$). A coarse grid with the resolution of 128 cells in stream-wise, 32 in wall-normal and 32 in span-wise directions. Periodicity was considered in stream-wise and span-wise directions. Wall layer model was applied using standard Smagorinsky. Then after reaching a steady state, an inflow was obtained for the hill case with the same resolution in $yz$.

The result of this simulation revealed that the current wall layer model was not able to capture separation of flow, unless if the grid is stretched near the wall so that the distance of the nearest computational node to the wall is less than or equal to 7 in wall unit. Also the case in which the first centroid was at $y^+_c(1) = 4$ displayed the best
results. Figure 5.2 shows the comparison between the simulation of cases in which the first centroids are at \( y^+(1) = 4 \) and \( y^+(1) = 7 \), compared with the experiment done by Khurshudyan et al. [20]. For both cases in our simulation, \( \Delta x^+ \approx 50 \), \( \Delta z^+ \approx 37 \) and \( \Delta y^+_{\text{max}} \approx 74 \). The simulations were carried out using a fixed Courant number equal to 0.2, and \( \Delta t \) is changing in every simulation to obtain the fixed Courant number. Courant-Friedrichs-Lewy (CFL) condition is defined as below.

\[
CFL = \left( \frac{|u_1|}{\Delta x} + \frac{|u_2|}{\Delta y} + \frac{|u_3|}{\Delta z} \right) = \left( |U_1| + |U_2| + |U_3| \right) \frac{\Delta t}{J^{-1}}.
\]  

(5.3)

Where \( u_i \) are Cartesian velocities and \( U_i \) are contravariant fluxes. The current wall layer model is able to capture flow separation when the first computational node is located in the viscous layer. However, it is not able to capture start point of separation at \( x = 0.5 \), and separation is a bit underestimated, finally the reattachment point is predicted well.

Stream-wise velocity fluctuations in fig. 5.2b show an undervaluation in the case with \( y^+(1) = 7 \) before the flow reaching to the hill. This discrepancy can be due to the fact that the first centroid in this case is not fine enough to stay exactly inside the viscous layer, therefore it does not predict the fluctuations well near wall. The undervalued fluctuations near wall lead to an under-prediction of turbulence propagation from the wall, and this values is larger far from the wall.

In the next section the optimization which was carried out to increase accuracy of the current wall layer model in order to capture flow separation when the first centroid is located in logarithmic region is explained.

### 5.2 Wall layer model optimization for body-fitted cases

The wall function which was presented, works very well in attached flows, but in detached flows stretched mesh is required near the wall so that the first centroid is set in the viscous layer. To improve the wall function a uniform coarse mesh was generated with 20 cells in wall normal direction in which the first computational node situated in the logarithmic region at \( y^+(1) \approx 30 \).

Cabot and Moin [6] applied wall layer model on LES to simulate flow over a backward facing step. They considered a zonal approach using thin boundary layer equations (TBLE) in the inner layer and LES (dynamic SGS model) in the outer region. In this way they could reduce the number of cells in wall normal direction from a stretched grid which was used for the previous work using resolved LES, to 8 uniform cells from the bottom wall to the half height of the step.
5.2. WALL LAYER MODEL OPTIMIZATION FOR BODY-FITTED CASES

Figure 5.3: Domain grid with resolution of $96 \times 20 \times 32$ cells in stream-wise, wall normal and span-wise directions respectively, for simulation of flow over hill using dynamic $k$.

Cabot and Moin [6] modified the Von Karman constant dynamically to equate the stress predicted by TBLE in the inner layer ($ky\widehat{u_iu_j}$) in a least-square sense to the total resolved and SGS stresses computed by LES in the outer region ($-\widehat{u_iu_j} - \widehat{\tau_{ij}}$). They used this dynamic $k$ to calculate eddy viscosity for the inner region, $\nu_t = kyu_D$, $D = [1 - \exp(-y^+/A^+)]^2$ in which $A^+ = 17$, but in that case since $y^+ \gg A^+$ they considered $D$ as unity. The dynamic $k$ was calculated as below.

$$k \sim -\frac{<y\widehat{u_iu_j}\widehat{S_{ij}}(\widehat{u_iu_j}) + \widehat{\tau_{ij}}>}{<y^2\widehat{u_iu_j}\widehat{S_{ij}}\widehat{S_{ij}}>}, \quad (5.4)$$

in which $<>$ denotes span-wise direction averaging. Instead of the zonal approach, we used wall layer model with dynamic Smagorinsky SGS model on a uniform coarse grid, and only applied this dynamic $k$ on our LES model to compute $u_r$ and then to calculate strain rate tensors as it was described in chapter 4 section 4.1. First it was tested on a periodic open channel flow with the resolution of $48 \times 20 \times 32$ grids in stream-wise, wall-normal and span-wise directions respectively, and dimension of $7.12h \times h \times h$ in which $h = 1 \text{ m}$.

Using 20 cells in wall normal direction allocates the near wall computational nodes at theoretical $y^+ \approx 30$, and a coefficient obtained for the open channel flow so that $k$ value in equation (5.4) becomes 0.41, which is the Von Karman constant. Then from the open channel flow, an inflow was obtained for the hill case.

A very coarse grid with resolution of $96 \times 20 \times 32$ cells in stream-wise, wall normal and span-wise directions was generated to carry out the flow simulation over hill applying dynamic $k$, as it was mentioned before with the same cross-sectional resolution of the channel to use inflow. The grid domain is shown in fig. 5.3. In this case, the grid spacing in wall units is $\Delta x^+ \approx 88$, $\Delta y^+ \approx 60$, $\Delta z^+ \approx 75$, using a fixed Courant number equal to 0.2.

For the open channel flow, a plane average approach to calculate dynamic $k$ values never gives a negative amount for $k$, while span-wise averaging at some time steps gives a negative value at few points which causes instability. The value of $k$ also can not be zero since it is used in denominator to calculate friction velocity and also strain...
rate tensors (section 4.1), therefore a positive value must be considered as a minimum. Setting the minimum value of 0.06 was enough to overcome this issue. Also bigger value than 0.06 was tested to check whether the results are sensitive to this lower bound, consequently it did not affect on the results, hence the method is robust from this aspect.

Figure 5.4a shows temporal and span-wise averaged velocity profile at different positions in stream-wise direction. According to the experiment [20], separation starts at $x = 0.5a$. As it is obvious in fig. 5.4a, our resolution is too low, and the first computational node is out of the separation region, therefore it is reasonable that we can not observe separation there.

Prediction for reattachment point is accurate in our simulation, at $x = 2a$ separation is captured and finally at $x = 3a$ there is the reattachment point. In comparison with resolved LES done by Chaudhari et al. [7] who applied a high resolution grid with $495 \times 70 \times 136$ cells in stream-wise, vertical and span-wise directions to simulate flow
5.3 Conclusion of Wall layer model in body-fitted cases

The equilibrium stress wall layer model which is based on law of the wall worked well in attached flows with uniform coarse grid, while this wall function can capture separation if the first computational node near wall is located in viscous layer. For simulation of separated flow over a single hill, locating the near wall centroid at $y_c^+(1) = 4$ displayed
the best result. Therefore a grid stretching is required to simulate separated flows.

Improving the wall layer model and using dynamic $k$ instead of Von Karman constant made the wall function able to capture separation in a uniform coarse grid in which the first computational node was located at $y^+ \approx 30$. A larger $k$ than the Von Karman constant downhill and in separation region was needed to capture separation. Figure 5.6 shows instantaneous values of dynamic $k$ in a stream-wise line over the hill.

According to this figure, three or four times bigger value than Von Karman constant near hill crest and also in separation region is observed. Since dynamic $k$ is in denominator of velocity, the large values over the hill decreases velocity and makes it possible to capture separation, while in simulation of flow over backward step by Cabot and Moin [6], a smaller dynamic $k$ than Von Karman constant was required to match stress calculated from TBLE in inner layer and the one computed by LES in our region.

The wall layer model with dynamic $k$ was also tested on different grid resolutions. The results for finer grids like 32 cells in vertical direction was not very good and separation was a bit over-estimated since the first computational node was located in buffer layer. Also with a coarser grid (16 cells in wall normal direction) separation was captured, but since the near wall node was far from wall, separation was captured from $x = 1.25a$. In conclusion the wall layer model using dynamic $k$ had the best accuracy when the first centroid was located in the logarithmic region.

This work was done to improve wall layer model in body-fitted grids in absence of immersed boundaries. In most of engineering and environmental applications geometries are complex and in many cases it is not practical to use a structured grid following the geometry. For these cases LES – COAST can treat the complex geometries as immersed boundaries. The advantage of immersed boundary methodology in this solver...
is that this methodology is directly applied on LES (Roman et al. [30] and [31]). It has also some disadvantages in separated flows as it will be described in the next chapter. Optimizations in both attached and detached flows are also carried out.
CHAPTER 5. IMPLEMENTATION AND OPTIMIZATION OF BODY-FITTED
Chapter 6

Implementation and optimization of Immersed boundary methodology

In addition to the body-fitted case, the hill geometry was created with GID software and was used as immersed boundary. The inflow for this case was obtained from a fully developed channel flow with an immersed boundary surface as the bottom wall, and triangular surface mesh was generated on the immersed boundary.

A domain with 6.675 m length in stream-wise, 1 m off-wall height (the height above the IB surface), and 1 m width was considered first with 160 grid cells in x, 36 cells in y which 32 of them located above the IB surface, and 32 cells in z directions. Two different types of domain grids were generated; a normal orthogonal grid (Cartesian grid) and a curvilinear grid so that its bottom following the hill geometry (see fig. 6.1).

The result of the simulations for both cases showed that the current wall layer model in IBM was unable to capture separation with this resolution. Changing the vertical resolution from 32 to 61 cells above immersed boundary surface, located the first computational node in viscous layer at $y^+ = 4.84$ (fig. 6.1). Although the case with orthogonal grid showed a bit better result than the curvilinear one, but accuracy of the model for detached flow was not acceptable. The case with curvilinear mesh was not able to display separation at all. Mean velocity profile is shown in fig. 6.2.
6.1 Calibration of the Immersed boundary method

In order to check accuracy of the current IBM, a plane channel considered with the same size and resolution of the channel we used for body-fitted case, with the resolution of $48 \times 20 \times 32$ grids in stream-wise, wall-normal and span-wise directions respectively, and dimension of $7.12h \times 1h \times 2h$ in which $h = 1 \, m$. Instead of the lower wall, an immersed boundary was applied and the simulation carried out with imposing a constant pressure gradient $(dp/dx = 1)$, at $Re_\tau = 2000$, so the first centroid for both cases were located at $y^+ = 50$. Then the results for both IB and the body-fitted cases compared with each other.

Considering non-scaled averaged velocity for both cases, the channel with immersed
6.1. Calibration of the Immersed Boundary Method

Figure 6.2: Mean stream-wise velocity of flow over hill for orthogonal mesh using IB versus experiment by Khurshudyan et al. [20].

Figure 6.3: Five different channels using immersed boundary as lower wall in different positions, cases 1 to 5 in order from left to right. Filled square displays IB node.

boundary underestimated velocity in comparison with the body fitted case, at all points. The shear velocity was calculated from averaged velocity at the first off-wall centroid by Newton-Raphson iterative method. While expecting the value of shear velocity and also wall shear stress to be close to 1 for the case with immersed boundary based on theory, approximately 16% underestimation was observed. Consequently there was a momentum loss due to the undervaluation of the wall shear stress.

After this observation, several cases of open channel geometries were created with the same size, and very close resolution, only the immersed boundary surface was moved slightly to check whether the IBM is geometry dependant. Four cases in which the first off-wall centroid is located in the logarithmic region, and one case in viscous layer. Immersed boundary positions for five cases are displayed in Fig. 6.3 and also details are explained in table 6.1. The horizontal grid spacing in wall units for all cases is $\Delta x^+ \approx 297$ and $\Delta z^+ \approx 125$.

Thereafter the simulation was carried out for all cases at $Re_\tau = 2000$, with the same boundary conditions. The results showed an underestimation of friction velocity for
cases 1 to 4 in which the IB node was set in the logarithmic region, and overestimation of shear velocity for case 1 which has the IB node in viscous layer (see table 6.1).

Despite of the shear velocity deviation, non-scaled velocity compared to law of the wall showed a good accuracy especially for the first four cases. The comparison of all cases with law of the wall and also DNS of closed channel flow done by Hoyas and Jimenez [17] is shown in the fig. 6.5a. A calibration of the IBM was carried out to avoid momentum loss. Therefore the wall shear stress had to be equal to unity, meaning that for these cases the friction velocity calculated from mean velocity at the IB nodes must be very close to the theoretical value, which is one.

For this purpose, we started to change the coefficient used to calculate eddy viscosity at the IB nodes \((C_w)\) in equation (4.14), to reach the ideal value. Following this procedure and changing the coefficient step by step in every simulation was giving a slight difference in the value of shear velocity, concluding that our IBM is robust.

Finally after varying the coefficient for all five cases in a wide range, we were able to

Table 6.1: Different geometries description of IB cases and shear velocity obtained from simulation.

<table>
<thead>
<tr>
<th>Case</th>
<th>IB surface position</th>
<th>(d^+_{IB})</th>
<th>(u_\tau)</th>
<th>(\Delta y^+)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>just above centroid</td>
<td>101</td>
<td>0.8883</td>
<td>109</td>
</tr>
<tr>
<td>2</td>
<td>between centroid and grid line</td>
<td>82</td>
<td>0.8816</td>
<td>110</td>
</tr>
<tr>
<td>3</td>
<td>just above grid line</td>
<td>43.5</td>
<td>0.8541</td>
<td>112</td>
</tr>
<tr>
<td>4</td>
<td>overlapping grid line</td>
<td>50</td>
<td>0.8393</td>
<td>100</td>
</tr>
<tr>
<td>5</td>
<td>just below centroid</td>
<td>5</td>
<td>1.2740</td>
<td>114</td>
</tr>
</tbody>
</table>
6.1. Calibration of the Immersed Boundary Method

(a) Mean velocity for IBM cases before calibration versus law of the wall, and DNS of closed channel.

(b) Mean velocity for IBM cases after calibration versus law of the wall and DNS of closed channel.

Figure 6.5: Mean velocity for IBM cases before and after calibration versus law of the wall and DNS of closed channel flow at $Re_\tau = 2000$ by Hoyas and Jimenes [17].

find an ideal coefficient which had to be used to calculate the eddy viscosity at the $IB$ nodes in order to conserve momentum of the flow. Table 6.2 shows the ideal coefficients and friction velocities obtained after running the simulations for all five cases.

The simulations also were repeated at $Re_\tau = 4000$ to check the accuracy of the calibration, concluding that it had an acceptable exactness.

After finding the proper coefficient for each case, this value was considered as a function of the ratio of $IB$ node distance from the immersed boundary surface ($d_{IB}$) over the grid spacing in vertical direction ($dy$), and a cubic line was properly fitted to the calibrated values (see figure 6.4). The maximum difference of the coefficient calculated from this cubic curve was 0.0665%, showing the accuracy of this cubic fitting is high.

Consequently the coefficient could be written as a function of the geometrical aspect
ratio \( (d_{IB}/dy) \) which was in the interval of zero to one. The equation of cubic curve which was fitted to the points is written below.

\[
C_c = -6.9576 \left( \frac{d_{IB}}{dy} \right)^3 + 15.051 \left( \frac{d_{IB}}{dy} \right)^2 - 10.902 \left( \frac{d_{IB}}{dy} \right) + 3.8493 \quad (6.1)
\]

The non-dimensional mean velocity profiles after calibration for all cases are shown in fig. 6.5b. All cases are non-dimensionalized by the shear velocity obtained from mean velocity at the IB nodes based on law of the wall. An improvement can be observed after calibration, specially for case 5 in which the IB node is located close to the immersed boundary. Finally the RANS-like eddy viscosity at the IB nodes can be calculated from the calibrated coefficient \( C_c \), which was obtained from the cubic fitting.

\[
\nu_T = C_c ku_\tau d_{IB} \quad (6.2)
\]

Calibrating the coefficient to calculate eddy viscosity, we were able to improve the wall shear stress computed from mean velocity at IB nodes in order to conserve momentum in our flow simulation, and therefore the velocity profile had a higher accuracy.

The results of the simulations for all cases show that the mean velocity and root mean square of velocity fluctuations are in a good agreement with the law of the wall and also DNS of plane channel flow done by Hoyas and Jimenez [17] for a closed channel at \( Re_\tau = 2000 \), only for the cases 3 and 4 in which IB nodes are in the beginning of log region \((d_{IB}^+ \leq 50)\) there is a deviation of the mean velocity profile from log law (fig. 6.5b).

The root mean square of velocity fluctuations are displayed in fig. 6.6. Fluctuations of the horizontal velocities are in a good agreement with the DNS data, while the vertical velocity fluctuations are under-estimated near wall. Near the free surface, we have a decline in vertical velocity fluctuations since it must be zero at the water surface.

Table 6.2: Ideal coefficient for IB cases and shear velocity obtained using this coefficient in simulation.

<table>
<thead>
<tr>
<th>Case</th>
<th>( d_{IB}/dy )</th>
<th>coefficient(( C_{ideal} ))</th>
<th>( u_\tau )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.93318</td>
<td>1.13</td>
<td>0.9987</td>
</tr>
<tr>
<td>2</td>
<td>0.74818</td>
<td>1.20</td>
<td>1.0043</td>
</tr>
<tr>
<td>3</td>
<td>0.38909</td>
<td>1.47</td>
<td>0.9966</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>1.3</td>
<td>0.9974</td>
</tr>
<tr>
<td>5</td>
<td>0.04386</td>
<td>3.4</td>
<td>0.9942</td>
</tr>
</tbody>
</table>
6.1. CALIBRATION OF THE IMMERSED BOUNDARY METHOD

(a) Stream-wise velocity fluctuations.

(b) Vertical velocity fluctuations.

(c) Span-wise velocity fluctuations.

Figure 6.6: Velocity fluctuations for the calibrated IBM compared to DNS of closed channel flow at $Re_\tau = 2000$ by Hoyas and Jimenes [17].

Computing the Reynolds shear stress $<u'v'>$ in which $<>$ denotes temporal and plane average, showed a gap between the Reynolds shear stress in global references and the value calculated from our simulation using calibrated IBM for case 4, as it is shown in fig. 6.7. This figure shows non-dimensional Reynolds shear stress by shear velocity obtained from mean velocity at the IB nodes based on law of the wall.

Although our wall layer model had a very good accuracy to predict wall shear stress, but it underestimated the fluctuations like most of the wall layer models. At this stage we decided to add some random fluctuations near the wall to improve our wall layer model. In the next section the details of these random fluctuations are described.
CHAPTER 6. IMPLEMENTATION AND OPTIMIZATION OF IBM

Figure 6.7: Reynolds shear stresses in global coordinates compared to our calibrated IBM for case 4 and DNS of closed channel flow by Hoyas and Jimenez [17].

6.2 IBM optimization for attached flows

As it was discussed in the end of last section, our calibrated IBM underestimated velocity fluctuations in vertical direction and consequently Reynolds shear stresses. Taylor and Sarkar [38] used some random stochastic forces in wall normal direction after they found that near wall model (NWM) LES with dynamic eddy viscosity model (DEVM) underrates vertical velocity fluctuations.

This force is applied as a term added to right hand side of momentum equation in wall normal direction to increase velocity fluctuations in this direction and controlling the Reynolds stress in order to converge it to the log law. This term was defined as multiplication of a random number between 0 and 1 by amplitude of the force.

\[ f_y(x, y, z) = \pm R \ast A(y), \]

(6.3)

The amplitude function \( A(y) \) can be obtained at each time step to set as summation of the amplitude at the last iteration and another term in order to converge the amplitude in proper direction and minimize the difference of the resolved shear stress and theoretical value based on logarithmic law.

\[ A(y)^{n+1} = A(y)^n + \frac{u_\tau \epsilon(y)}{\tau}, \]

(6.4)

in which the error function can be written as:

\[ \epsilon(y) = \frac{k y}{u_\tau} \left( \frac{d(u)^2}{dy} + \frac{d(u)^2}{dy} \right)^{\frac{1}{2}} - 1, \]

(6.5)
6.2. IBM OPTIMIZATION FOR ATTACHED FLOWS

Figure 6.8: Mean velocity profile before and after adding stochastic forces for case 4 compared to log law and DNS of closed channel flow by Hoyas and Jimenez [17].

where \( \tau \) is relaxation time. This approach is correct if the first computational node is in logarithmic region since in equation (6.5) the error is established upon \( ky/u_\tau \) which is the theoretical resolved shear stress based on logarithmic law. Finally sign of the force function is computed to decline the correlation of stream-wise and vertical velocity fluctuations \((u'\text{ and } v')\) if the error is positive and enhance this correlation if the error is negative.

\[
\text{sgn}(f_y(x, y, z)) = -\text{sgn}(\frac{d\langle u_s \rangle}{dy}) \times \text{sgn}(\epsilon(y)) \times \text{sgn}(u'_s(x, y, z)),
\]

where \( u_s \) is velocity in the direction of mean wall shear stress. For example considering the first off wall computational node in which \( d\langle u_s \rangle/dy \) is positive in channel flow, if the mean shear stress is underestimated, means that the error function is less than zero, hence the sign of stochastic force is the same as \( u'_s \), i.e. the force is in such a way to pull the low speed flow toward the wall and push the high speed flow away from the wall.

In contrast if the mean shear stress is underrated, the error function has a positive value and then the sign of stochastic force is different from \( u'_s \) and in this situation the force acts to pull the high speed flow toward the wall and push the low speed flow far from the wall.

We started to impose the stochastic random force on case 4. Since \( IB \) nodes were located in logarithmic region, they were interpolated based on logarithmic law from projection points \( PP \), and therefore adding this force to the first two nodes did not improve the velocity profile. Then considering one more point to impose the forcing term on, showed an improvement of the mean velocity profile (fig. 6.8).

Adding stochastic forces to the first three off-wall (above the immersed boundary)
computational nodes in vertical direction, increased the Reynolds shear stresses which was shown in fig. 6.7 and consequently improved the velocity profile which was obtained from calibrated IBM (fig. 6.8).

The relaxation time played an important role in the simulation. It has to be large enough to let the flow adapt itself to the force. In the other hand, if the relaxation time is too large the effect of force is less. In our simulations, $0.0006 \frac{\delta}{u} \leq \tau \leq 0.002 \frac{\delta}{u}$ gave the best results. The values larger than $0.002 \frac{\delta}{u}$ increased the velocity continuously since the flow did not have enough time to adjust itself to the force, and the values less than $0.0006 \frac{\delta}{u}$ only improved a bit the velocity profile.

In conclusion, implementing a forcing term in the right hand side of the momentum equation in wall normal direction for the first three points, including a multiplication of a random number between 0 and 1, and an amplitude which was set dynamically at each time step in order to guarantee that the velocity at these three points converging to the logarithmic law improved our wall layer model of calibrated IBM for attached flow. An error was calculated at each time step as the difference between resolved and logarithmic shear stresses, and finally the sign of this forcing term was determined to minimize the error.

This method works perfectly when the IB node is located in the logarithmic region and in attached flows since we expect to have a logarithmic relation for the velocity. In the next section, flow over hill is discussed which is a very challenging problem specially where immersed boundaries are used.

6.3 IBM Optimization in detached flows

The IBM was tested to simulate the flow over a single hill but the flow separation was not captured. Also trying another case in which the flow moves over periodic hills [39] did not show flow separation. Even restarting from a laminar flow in which there was flow separation was not effective, and separation started disappearing from downhill to the end of the separation region. To understand why the IBM had this weakness, the theory of separation phenomena must be carefully perceived.

In a plane channel flow the external pressure gradient is zero. When flow passes over a curvature solid, the outer flow streamlines converge at the highest point upstream, resulting in an augment of the free stream velocity and leading to a fall pressure in stream-wise direction, while downstream of the highest point the streamlines diverge, leading to a decline of free stream velocity and increasing the pressure. In order to understand the theory, we can write two dimensional boundary layer equations as
6.3. IBM OPTIMIZATION IN DETACHED FLOWS

\[ \frac{u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2}. \]  \hspace{1cm} (6.7)

To realize the flow formulation for separation, since at the wall with no slip boundary condition, the horizontal and wall normal velocities are zero, the first two terms are neglected. Therefore pressure gradient and second order vertical derivative of horizontal velocity are equal.

\[ \nu \left( \frac{\partial^2 u}{\partial y^2} \right)_{wall} = \frac{1}{\rho} \frac{\partial p}{\partial x}. \]  \hspace{1cm} (6.8)

When the pressure gradient of the external stream is negative (favourable), the second derivative of velocity \( \frac{\partial^2 u}{\partial y^2} \) is also negative in this region, meaning that slope of the profile of velocity gradient \( \frac{\partial u}{\partial y} \) is negative. Then going farther from the wall, just before joining the outer region at the top part of the boundary layer, this term goes to zero since it must continuously fit to the outer region. Concluding that the second derivative of velocity at the wall and also inside the boundary layer has the same sign.

In contrast when the flow stream has reverse (unfavourable) pressure gradient, the second derivative of velocity is positive therefore there is a change of sign of the velocity curvature inside the boundary layer. At a point called inflection, the second derivative of velocity becomes zero, \( \frac{\partial^2 u}{\partial y^2} = 0 \). From continuity equation it can be seen that unfavourable pressure gradient contributes to an increase in boundary layer thickness.
Therefore decelerating pressure gradient creates an inflection point in boundary layer and rises quickly. Presence of inflection point signifies a region next to the wall in which the flow slows down. If the reverse pressure gradient is strong enough, the flow next to the wall changes direction to opposite side. The reverse flow meets the forward flow at separation point (S point in fig. 6.9). The separation point is the boundary between the forward and reverse flows, and stress at this point is equal to zero.

\[
\left( \frac{\partial u}{\partial y} \right)_{\text{wall}} = 0. \tag{6.9}
\]

As it was described for a flow over a curvature solid, adverse pressure gradient makes the flow have an inflection point, and if this decelerating pressure gradient is big enough, velocity of the flow near wall goes to zero and then to negative values signifying separation. In our IBM, velocity at the IB nodes are always calculated from friction velocity at projection points. It means that velocity of the IB is always in the same direction of the velocity at projection point.

Therefore the reason that our calibrated IBM does not capture separation of the flow over hill is that the star point of separation where the flow near wall changes direction is not regarded. For this reason, we started to derive a theory from boundary layer equation at wall for calculating the velocity at IB nodes:

\[
\nu_T \left( \frac{\partial^2 u}{\partial y^2} \right)_{IB} \approx \frac{1}{\rho} \left( \frac{\partial p}{\partial x} \right)_{IB}^{IB}. \tag{6.10}
\]

Using Central Difference Scheme (CDS) in order to discretize the second derivative of velocity for a non-uniform grid [12], considering PP, IB and IP nodes, we can write:

\[
\left( \frac{\partial^2 u}{\partial y^2} \right)_{IB} \approx \frac{u_{PP}(d_{IB}) + u_{IP}(d_{PP-IB}) - u_{IB}(d_{PP})}{\frac{1}{2}(d_{PP})(d_{PP-IB})(d_{IB})}, \tag{6.11}
\]

in which \(d_{PP-IB}\) is the distance between IB and PP points. Finally the streamwise tangential velocity at the IB can be written as a function of tangential pressure gradient instead of friction velocity;

\[
u_T \left( \frac{1}{\rho} \frac{\partial p}{\partial x} \right)_{IB}^{IB} = C \left( \frac{\partial p}{\partial x} \right)_{IB}^{IB} \frac{(d_{PP-IB})(d_{IB})}{\nu_T}, \tag{6.12}
\]

where the pressure gradient is the tangential pressure gradient at IB node, and the eddy viscosity is also the calibrated value obtained from equation (6.2).

Using a coefficient (C) in order of \(10^{-3}\) inside the second term in which there is the pressure gradient at IB, can rescale the large values obtaining from big pressure gradient dividing by small values of turbulent eddy viscosity. Many tests carried out to
6.3. IBM OPTIMIZATION IN DETACHED FLOWS

(a) Mean velocity profiles for the cartesian and curvilinear grids at different locations in stream-wise direction; hill starts from $x = -a$ and ends at $x = a$.

(b) Root mean square of stream-wise velocity fluctuations.

Figure 6.10: The results for simulation of flow over single hill using new IBM scheme in Cartesian and curvilinear grids compared with experiment by Khurshudyan et al. [20].

find the best criteria for using this new scheme. Finally applying equation (6.12) where there are the conditions below gave the best results for simulating flow over single hill.

- $\left( \frac{\partial p}{\partial x} \right)_{IB} > 0$,
- $y(IP) - y(IP)_{\text{previous}} < -0.0001$.

Here the index previous is related to the previous point in stream-wise direction tangent to the immersed boundary surface. These two criteria mean that the new scheme to calculate tangential velocity at the $IB$ is used if the tangential pressure gradient at the $IB$ is unfavourable, and the immersed boundary surface is downward.

This new scheme was applied for simulation of atmospheric flow over two dimensional hill. First an open channel was constructed in which immersed boundary was considered as lower wall. After the channel flow reached a steady state, instantaneous
data was obtained from a cross sectional plane at different time steps. Then bottom of the domain including the hill shape was created as immersed boundary, and the data which was obtained from the channel flow, was used as inflow for simulation over the hill.

The simulation was carried out using two different grids; Cartesian and curvilinear meshes. Applying the new scheme, we were able to capture separation in the simulation with grid resolution of $128 \times 40 \times 32$ cells in stream-wise, wall normal and span-wise directions respectively. In the simulation for both grids, starting point of separation was predicted well at $x = 0.5a$. The reattachment point for both cases anticipated before $x = 2a$, therefore at this point the mean velocities are positive, although very small close to the immersed boundary surface. The mean velocity profiles for both grids were compared with the experiment by Khurshudyan et al. [20] as it is shown in fig. 6.10a.

Stream-wise velocity fluctuations in fig. 6.10b display a good agreement between the simulation for both grids and experiment. Although there is an overestimation of fluctuations after start point of separation, but the behaviour of velocity fluctuation profile for the simulations is similar to the experiment.

6.3.1 Flow simulation over 2D periodic hills

In addition to the case mentioned before, another test was also carried out using the new scheme. Case 81 of ERCOFTAC is flow over two dimensional periodic hills in a polynomial shape. Shape of the domain is shown in fig. 6.11. Inlet and outlet of the domain are at the top of the hills. Hills have the height of $h = 28 \text{ mm}$, and their crests are separated by $L_x = 9h$. The height of the channel is equal to $L_y = 3.035h$, and channel width is $L_z = 4.5h$. Shape of the hills are defined as the same as Case 18 of ERCOFTAC by Almeida et al. [1], in which the amplitude of the hills is $54 \text{ mm}$ and the spline follows a polynomial as defined below.
\[ h(x) = \begin{cases} 
\min(28, 20.80 + 0.00x + 0.006775x^2 - 0.00212453x^3) & \text{if } 0 \leq x \leq 9 \text{ mm} \\
25.07356 + 0.97548x - 0.1016116x^2 + 0.001889795x^3 & \text{if } 9 < x \leq 14 \text{ mm} \\
25.7960 + 0.820669x - 0.0905537x^2 + 0.001626511x^3 & \text{if } 14 < x \leq 20 \text{ mm} \\
4.046435 - 1.379582x + 0.019458845x^2 - 0.000207x^3 & \text{if } 20 < x \leq 30 \text{ mm} \\
17.92461 + 0.087439x - 0.0556736x^2 + 0.00062777x^3 & \text{if } 30 < x \leq 40 \text{ mm} \\
\max(0, 56.39 - 2.01052x + 0.016449x^2 + 0.000027x^3) & \text{if } 40 < x \leq 54 \text{ mm} \\
\end{cases} \]

Bottom of the domain is displayed in fig. 6.13 was created with GID software and a
triangular surface mesh was generated on this part to be treated as immersed boundary.
Then computational domain was created, with generation of Cartesian and curvilinear
grids with different resolutions (see fig. 6.12). First the domain with grid resolution of
96 \times 64 \times 32 cells out of immersed boundary in stream-wise, wall normal and span-wise
directions respectively was considered, which was the coarsest grid in Chen et al. [8]
who simulated flow over periodic hills using immersed boundary and applied a zonal
approach (TLM); TBLE close to immersed boundary and LES in farther region.

Reynolds number based on hill height and bulk velocity on top of the first hill is
equal to: \( Re = \frac{U_b h}{\nu} = 10595 \), where \( \nu \) is laminar viscosity. The flow is periodic in \( x \)
and \( z \) directions, using immersed boundary at bottom and free surface at top.

The result for the case with Cartesian grid showed an overestimation of separation,
while the case with curvilinear grid predicted separation well. Observing these results,
another test was carried out using a higher resolution in Cartesian grid and a lower
resolution in curvilinear mesh. The curvilinear case applying 32 off-wall cells in vertical
direction also over-predicted separation region, while the simulation diverged in
Cartesian grid with 76 cells in wall normal direction due to the large negative values
of tangential velocity at IB nodes obtained from our new scheme.

Many different tests were done first on Cartesian grid to understand the reason why
it diverges using the new scheme on higher vertical resolution than 64 cells. Finally
adding one more condition to the criteria for using the new scheme solved this problem.
Since in Cartesian grid the distance of IB nodes from immersed boundary surface (\( d_{IB} \))
has a large variation from one cell to another, in comparison to curvilinear grid in which
the range of these variations is not much (fig. 6.13), the tangential velocity at IB nodes
in equation (6.12) can be negatively large enough to over-predict the separation and
also diverge the simulation in some cases.

The flow simulation over periodic hills applying Cartesian grid, using the new
scheme gave the best result when equation (6.12) was employed at the positions with
these criteria below.

- \( \frac{\partial p}{\partial x} \bigg|_{IB} > 0 \),
- \( y(IP) - y(IP)_{\text{previous}} < -0.0001 \),
- \( d_{IB}^+ < 60 \).

First it was tested on a grid with resolution of 96 × 76 × 34 cells in stream-wise, wall
normal and span-wise directions respectively, in which the grid spacing in wall units
was \( \Delta y^+ \approx 88 \) and \( IB \) node at \( d_{IB}^+ = 44 \) in the middle of channel between the hills.
Then lowering the resolution, also with using 44 cells in vertical direction with grid
spacing of \( \Delta y^+ \approx 153 \) and \( IB \) node location at \( d_{IB}^+ = 76 \) in the middle of channel, the
result was pretty good.

Figure 6.14 displays the results for our simulation over periodic hills applying our
new scheme on Cartesian grids with 44 and 76 cells in vertical direction, compared
to resolved LES by Temmerman and Leschziner [39] at ten different downstream lo-
6.3. IBM OPTIMIZATION IN DETACHED FLOWS

Figure 6.13: Near wall nodes downhill of the period hills grid; left: Curvilinear and right: Cartesian mesh, circles show IB nodes, black cubes projection points, and the red spheres IP nodes.

cations, the data for resolved LES is provided by ERCOFTAC, velocities are non-dimensionalized by $U_{\text{bulk}}$ which is the bulk velocity on the first hill crest, also Reynolds stress and turbulent kinetic energy are non-dimensionalized by $U_{\text{bulk}}^2$.

Figure 6.14a shows mean stream-wise velocity (averaged in time and span-wise direction) at different positions compared to the resolved LES by Temmerman and Leschziner [39]. Mean velocity profile for Cartesian grid using the new scheme was in a good agreement with the resolved LES on the whole. Although the mean velocity at $x = 0.5h$ is matching the profile obtained from resolved LES, but the velocity is not negative at the IB node. Separation is captured with both 44 and 76 vertical off-wall cells even at $x = 5h$, where is very close to reattachment point. With both resolutions the reattachment point was predicted accurately.

Mean vertical velocity in fig. 6.14b is a bit overestimated in the finer case and underrated close to the wall on top of the hill ($x = 0.05h$). This quantity downhill as well as uphill is slightly underestimated in both grids, a bit more near wall in the coarser mesh. In other regions it is in a good agreement with resolved LES.

Figure 6.14c shows a small undervaluation of Reynolds shear stress for the finer and very small overestimation in the coarser grid downhill, and then a close behaviour in the finer grid and resolved LES at other points. Reynolds shear stress is marginally overestimated at $x = 2h$ in coarser grid and then undervalued at $x = 3h$ in this case. This quantity is also slightly overrated uphill in both cases, but generally it shows the same behaviour of resolved LES.

As it is illustrated in fig. 6.14d, turbulent kinetic energy in both cases is also predicted the same behaviour of the resolved LES, only with an overestimation uphill, hill crest and downhill in the finer grid and a marginal undervaluation in the coarser grid after the hill.
In order to compare relative pressure on the immersed boundary surface through the whole domain, pressure coefficient was also computed at the IB nodes as below.

\[ C_p = \frac{p - p_0}{\frac{1}{2} \rho U_0^2}. \]  

(6.14)

In which \( p_0 \) is the reference pressure, in this case is pressure at top of the first hill, and \( U_0 \) is also the reference velocity, here it is considered as the bulk velocity at the first hill crest which has been used to non-dimensionalize the mean velocities, Reynolds stress and turbulent kinetic energy. In addition to the pressure coefficient, friction coefficient was also calculated at the IB nodes.

\[ C_f = \frac{\tau_w}{\frac{1}{2} \rho U_0^2}. \]  

(6.15)

To obtain the wall shear stress, first the tangential velocity (tangent to the immersed boundary surface) at each IB node was averaged in time and spa-wise, then considering the distance of the IB node from immersed boundary surface \( d_{IB} \), friction velocity was calculated from linear relation or Newton-Raphson iterative method based on logarithmic law depending on \( d_{IB}^+ \), and then wall shear stress was computed from the shear velocity.

Figure 6.16 shows drag and pressure coefficients for the simulation in Cartesian mesh compared with resolved LES by Frohlich et al. [13]. Data for the resolved LES collected from NASA Langley Research Center.

The simulation overrates drag coefficient on top of the hill. In resolved LES this coefficient changes sign downhill at \( x \approx 0.22h \), while in our simulation with the finer grid \( C_f \) becomes negative at \( x \approx 0.53h \) and in the coarser grid this happens at \( x \approx 0.64h \), both after the starting point of separation the mean stream-wise velocity at the IB node is not negative at \( x = 0.5h \) in fig. 6.14a for both cases.

In separation region also an over-prediction is displayed, the resolved LES shows the drag coefficient changing sign at reattachment point at \( x \approx 4.69h \) while in the simulation \( C_f \) changes sign a bit before, the finer grid at \( x \approx 4.24h \) and the coarser grid at \( x \approx 4.5h \). Then simulation underestimates the drag coefficient uphill till \( x \approx 8.74h \) (fig. 6.16a).

As it is displayed in fig. 6.16b, the coarser grid overestimates \( C_p \) in separation region, and after reattachment point is in a good agreement with the resolved LES, while the finer mesh under-predicts \( C_p \) everywhere except the region near the hill crest.

After Cartesian grid, the new scheme was tested on curvilinear grid with different
resolutions. The flow simulation over periodic hills in curvilinear grid showed the best results in different resolutions, applying the new scheme where:

- \( \left( \frac{\partial p}{\partial x} \right)_{IB} > 0 \),
- \( y(IP) - y(IP)_{previous} < -0.0001 \),
- \( d^+_{IB} < 90 \).

Using these criteria even the separation was captured with a very low grid resolution of \( 96 \times 32 \times 32 \) in stream-wise, wall normal and span-wise directions respectively, while applying Cartesian grid with this resolution, we were not able to predict separation. Figure 6.15 shows Mean stream-wise velocity, mean wall normal velocity, Reynolds shear stress and kinetic energy in curvilinear grid with two different vertical resolutions, one with 64 and another with 32 vertical off-wall cells, compared to resolved LES by Temmerman and Leschziner [39].

The reason for observing separation in curvilinear grid with less cells is that the grid spacing in Cartesian grid is the same everywhere, while it is less downhill in curvilinear case. For instance, curvilinear grid with 32 cells in vertical direction provided grid spacing at top of the hill equal to \( \Delta y^+_{hill \ crest} \approx 148 \) and between the hills \( \Delta y^+_{channel \ center} \approx 210 \), and in the finer mesh on \( \Delta y^+_{hill \ crest} \approx 72.5 \) and also \( \Delta y^+_{channel \ center} \approx 105 \). Therefore downhill region resolution plays an important role in this issue.

Mean velocity profile for both cases with 64 and 32 vertical off-wall cells is in a good agreement with resolved LES (fig. 6.15a). Velocity at the \( IB \) node at \( x = 0.5h \) where is the start of separation region, shows negative values correctly in the finer and coarser grids. Then there is a marginal over-prediction of stream-wise velocity in separation region close to the wall, such that at \( x = 4h \) which is very end of separation region, the velocity at the \( IB \) node is close to zero in both cases.

The two cases slightly under-predict mean vertical velocity downhill, the coarser grid overrates this quantity at the end of separation region and underestimates it uphill, while the finer grid overvalues it only uphill. Generally both cases behave the same as resolved LES as it can be seen in fig. 6.15b.

The coarser mesh undervalues Reynolds shear stress downhill as well as before reattachment point at \( x = 3h \), but overestimates it uphill (fig. 6.15c). Kinetic energy is overestimated downhill in the coarser grid as well as after flow reattachment, while it is partly undervalued at the top of the hill and also in the start of separation region in the finer grid as it is shown in fig. 6.15d.
Drag and pressure coefficients are illustrated in fig. 6.17 for the simulation over periodic hills using curvilinear grid with 64 and 32 vertical off-wall cells compared to the resolved LES done by Frohlich et al. [13]. Also in these cases there is an over-prediction of drag coefficient on top of the hill, and a delay to change sign to negative in comparison with the resolved LES. \( C_f \) in the finer grid changes sign at \( x \approx 0.48h \), a bit earlier than the coarser grid which starts having negative drag coefficient at \( x \approx 0.5h \) (fig. 6.17a).

The case with 32 vertical cells shows a sign change of \( C_f \) from negative to positive at \( x \approx 3.2h \), while the other case with 64 wall-normal cells displays this situation at \( x \approx 4.2h \) which is slightly before the resolved LES that experiencing this state at \( x \approx 4.69h \). In separation region an over-valuation for the drag coefficient is predicted in both simulation cases. After reattachment point there is a marginal underestimation of \( C_f \), and this discrepancy increases uphill.

Before starting separation downhill, simulation underrates pressure coefficient, then in separation region the finer grid shows a small over-valuation of \( C_p \) which after reattachment point matching with the resolved LES. The case with 32 vertical cells underpredicts pressure coefficient almost everywhere.

### 6.4 Conclusion for Immersed boundary methodology

Immersed boundary methodology proposed by Roman et al. [30] was used to simulate flow in channel flow and also over a single hill. This IBM showed a very small separation region using Cartesian grid and setting the \( IB \) node in viscous layer. Although the non-dimensional velocity profile of the channel flow had a good agreement with law of the wall specially when the \( IB \) node located in logarithmic region, but wall shear stress was underrated at \( IB \) node in logarithmic region and over-predicted in viscous layer, resulting momentum loss in our flow simulation.

A calibration of the eddy viscosity was carried out to predict wall shear stress more accurately and prevent the momentum loss. The calibrated IBM showed a high accuracy in prediction of wall shear stress in different cases with various immersed boundary positions with respect to the grid at \( Re_\tau = 2000 \) and also 4000.

The only weakness of the calibrated IBM was for cases in which the \( IB \) node was located in logarithmic region at \( d_{IB}^+ \leq 50 \). The reason for this weakness was undervaluing fluctuations in wall normal direction specially near wall. To optimize calibrated IBM in attached flows, a random stochastic forcing was applied to the first three near wall cells and in consequence Reynolds stress and velocity profile were improved.
Since velocity at the IB node always following the velocity at projection point, there was a difficulty to capture the start point of flow separation in simulating flow over the hill. To overcome this issue, a theory from boundary layer equation was derived to compute tangential stream-wise velocity at the IB node \(u_{IB}\) from pressure gradient instead of calculating it from shear velocity at projection point, where the pressure gradient is unfavourable and immersed boundary surface goes downward. Using this new scheme, we were able to capture separation in flow over single hill and also periodic hills.

In simulation of flow over the single hill, considering 20 cells which was also used in body-fitted case, was not enough since with this resolution the hill height was covered only by two fluid nodes. Considering 40 cells in wall normal direction, we were able to observe separation over single hill using Cartesian and also curvilinear grids. Start point of separation predicted well, but the flow reattached a bit earlier than the experiment. Comparing our simulation with resolved LES done by Chaudhari et al. \([7]\), accredited our model. With this resolution, the IB node was located in buffer layer at \(d_{IB}^+ \approx 15\).

Checking different resolutions proved that the new scheme should not be used in a very fine grid, as it did not work well using 80 cells in vertical direction for the single hill.

In addition to the single hill, we tested the new scheme on the simulation of flow over periodic hills. The single hill had a short height with respect to the domain height, therefore the grid spacing in wall units in this case was much smaller than the periodic hills. Since \(d_{IB}^+\) was much lower than 60, we did not need the third criterion \((d_{IB}^+ < 60)\). Also adding this criterion did not change the results obtained for the single hill. In contrast, since grid spacing in wall units was much higher in periodic hills, we had a limitation to use the new scheme. Adding \(d_{IB}^+ < 60\) criterion in Cartesian and \(d_{IB}^+ < 90\) in curvilinear grid to use the new scheme, we obtained very good results for simulation of flow over the periodic hills. All the simulations of either attached or detached flows, were carried out using a fixed Courant number equal to 0.2.

Previously Chen et al. \([8]\) simulated flow over periodic hills using immersed boundary, applying Turbulent Boundary Layer Equations (TBLE) near wall and LES farther on Cartesian meshes with different resolutions. The resolutions for their case were 96 \(\times\) 64 \(\times\) 32 cells in stream-wise, wall normal and span-wise directions with TBLE/LES matching point at averaged \(y^+ = 30\), and 192 \(\times\) 72 \(\times\) 64 cells with the matching point at \(y^+ = 15\). Comparing our results with them, we were able to predict friction coefficient closer to the resolved LES, and capture separation region better in overall with lower resolution, while they displayed a better pressure coefficient.

Table 6.3 displays resolution, separation and reattachment points in our IBM sim-
ulations compared with resolved LES by Frohlich et al. [13] and Wall Model LES by Chen et al. [8]. The advantage of our IBM is that we only reconstruct the velocity at the IB nodes without solving extra set of equations than LES. In this way, we were able to simulate separated flows well applying uniform coarse grid and using LES for all the domain. In addition to time and cost saving, we were able to propose a reliable method with high accuracy.
6.4. CONCLUSION FOR IMMERSED BOUNDARY METHODOLOGY

(a) Mean stream-wise velocity profiles.

(b) Mean vertical velocity profiles.

(c) Reynolds shear stress profiles.

(d) Kinetic energy.

Figure 6.14: Results for simulation of flow over periodic hills using Cartesian grid with two different vertical resolutions at different positions compared to the resolved LES done by Temmerman and Leschziner[39].
(a) Mean stream-wise velocity profiles.

(b) Mean vertical velocity profiles.

(c) Reynolds shear stress profiles.

(d) Kinetic energy.

Figure 6.15: Results for simulation of flow over periodic hills using curvilinear grid with two different vertical resolutions at different positions compared with the resolved LES done by Temmerman and Leschziner[39].
6.4. CONCLUSION FOR IMMERSED BOUNDARY METHODOLOGY

Figure 6.16: Friction and drag coefficients for simulation of flow over periodic hills using Cartesian grid compared with the resolved LES done by Frohlich et al.[13].

Figure 6.17: Friction and drag coefficients for simulation of flow over periodic hills using curvilinear grid compared with the resolved LES done by Frohlich et al.[13].
Table 6.3: Resolution, separation point ($x_s$) and reattachment point ($x_r$) in resolved LES [13], our IBM simulations, and Wall Model LES by Chen et al. [8].

<table>
<thead>
<tr>
<th>Case</th>
<th>resolution</th>
<th>$x_s$</th>
<th>$x_r$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resolved LES(Frohlich et al.)</td>
<td>$196 \times 128 \times 186$</td>
<td>0.224h</td>
<td>4.69h</td>
</tr>
<tr>
<td>IBM Cartesian ($n_2 = 44$)</td>
<td>$96 \times 44 \times 32$</td>
<td>0.64h</td>
<td>4.24h</td>
</tr>
<tr>
<td>IBM Cartesian ($n_2 = 76$)</td>
<td>$96 \times 76 \times 32$</td>
<td>0.53h</td>
<td>4.50h</td>
</tr>
<tr>
<td>IBM curvilinear ($n_2 = 32$)</td>
<td>$96 \times 32 \times 32$</td>
<td>0.50h</td>
<td>3.20h</td>
</tr>
<tr>
<td>IBM curvilinear ($n_2 = 64$)</td>
<td>$96 \times 64 \times 32$</td>
<td>0.48h</td>
<td>4.20h</td>
</tr>
<tr>
<td>WMLES(TBLE/LES at $y^+ = 30$)</td>
<td>$96 \times 64 \times 32$</td>
<td>0.65h</td>
<td>4.00h</td>
</tr>
<tr>
<td>WMLES(TBLE/LES at $y^+ = 15$)</td>
<td>$192 \times 72 \times 48$</td>
<td>0.50h</td>
<td>4.42h</td>
</tr>
</tbody>
</table>
Chapter 7

Applying LES on sea water circulation in Kaneohe bay

Coral reefs are important from ecological point of view. The sea water circulation over the coral reefs plays an important role in transportation and distribution of larval fish and corals. They are also important because of sediment transport and nutrient delivery to the reef organisms [22].

Physical formation of the bays with coral reefs are different from sandy beaches. For example in the bays with coral reefs, there is a tangible and steep change in the slope of bathymetry. Also the coral reefs are rough due to the reef organisms. There are not many numerical studies on predicting water circulation over the reefs comparing to the sandy beaches.

Waves usually break on the reefs, and the significant waves energy is dissipated because of the wave breaking and also friction on the sea bed. The result of the wave breaking is an increase in the elevation of mean water surface and a current passing over the reefs.

In order to understand sea water circulation in shallow water basins, numerical methods have been developed. With improving the capability of computers in high performance computing, LES has recently been implemented as a strong tool to illustrate the physical mechanism of interaction which happens in the basins in coastal areas.

Complexity of the bathymetry and coastline geometries can be handled by treating them as immersed boundaries. Immersed boundary methodology for LES – COAST was developed by Roman et al. [30] and [31], which is applied directly on LES without considering additional set of equations (chapter 4 section 4.2).

In semi-closed shallow waters, wind plays an important role in flow direction at the
sea free surface, and complexity of bathymetry and coastline make the flow turbulent in three dimensions. LES – COAST solver has been applied on Muggia bay in Trieste by Roman et al. [32] and also Petronio et al. [24], considering wind forcing, stratifications, and their effects on mixing in near-shore area. In addition to that, Galea et al. [14] used LES – COAST to simulate water mixing and renewals in Barcelona bay, Spain. They investigated currents and mixing to understand the physical behaviour of the sea water circulation with satisfactory results.

Previously some studies carried out on the sea water flow in Kaneohe bay. Jia et al. [18] investigated on the effects of ocean thermal energy conversion (OTEC) systems which are used as an energy source in Oahu, on near and far field sea water properties. The horizontal resolution for the Oahu regional model was around 1 kilometer with four layers in vertical direction. Lowe et al. [23] investigated on incident waves forcing in Kaneohe bay collecting 10 months experimental data. They considered some stations over the reef and also in channels and lagoon.

In other work, Lowe et al. [22] used a coupled waves-circulation numerical model to simulate the distribution of waves energy in presence of tide and wind within coral reef system. In the following chapter LES is applied to model sea water circulation, mixing and renewal in Kaneohe bay. The novelty of this work is that LES – COAST is used in such a challenging case for the first time. The coral reef with a minimum depth of less than 1 meter is located in presence of the deep lagoon with 10 to 15 meters depth.
7.1 Site description

Kaneohe bay is located in north-east side of Oahu island in Hawaii, where is windward. The bay is around 13 km long and 4 km wide. A coral reef is situated in the mouth of the bay and a lagoon is located behind the reef. The lagoon separates reef from shore, exchanging with the ocean through Ship Channel with approximately 12 m depth in north, and Sampan Channel in south with a mean depth of 5 meters (see fig. 7.1).

The sea water is influenced by wind from east and north-east and its corresponding waves. The bay consists a large reef with approximately 4 km length and 2 km width, and depth of the reef in most of the places is between 3 m to less than 1 meter. Incident waves with height of 1 to 3 m from ocean comes toward the fore-reef, and the break point is between fore-reef and reef flat.

Waves propagate after the break point and water comes over the reef and then goes to lagoon. In addition to waves, wind from east and north-east with speed of 5 to 10 m/s plays an important role in water circulation in this bay.

7.2 Computational domain

The aim of this simulation is to apply LES model for waves and wind driven water circulation in Kaneohe bay. In order to impose effect of waves in our simulation, the oceanic side boundary was fitted on the reef flat, very close to some stations in Lowe et al. [22] and [23]. Since our grid is not moving, we need to apply the effect of waves as velocity of current on the boundary. In addition to waves which can be considered on the boundary, wind forcing is also applied on the water surface at all regions.

For this purpose, a minimum depth of 1.2 m was considered over the coral reef and 1.5 m elsewhere. A grid with a fixed depth of 18 meter was generated with the resolution of 1024 × 32 × 768 cells in Easting (x), vertical (y) and Northing (z) directions respectively. A stretch was carried out to have maximum vertical grid spacing 1.4 m at the bottom and minimum grid spacing of 0.285 m at water surface. This stretching provided 4 cells above the reef flat in vertical direction. A horizontal stretch was also done to have a higher resolution on the reef. Grid spacing varied from 27 m on eastern
and western sides to 4.5 m on the reef. Also a variation from 11 m in the southern side to 4.5 m on the reef was applied in z direction. In this way a uniform horizontal resolution of $4.5 \times 4.5 \, m^2$ was set on the coral reef for the simulation. Coastline and bathymetry were regarded as immersed boundaries in the simulation. To apply the boundary conditions in north of the bay, some measurements of the flow are required. Here the boundary conditions are described.

### 7.3 Boundary conditions for simulation

For wind and waves, two references were regarded in order to establish real conditions in Kaneohe bay. Currents from the data of Oahu regional model by Jia et al. [18] was interpolated for our computational grid to understand the velocity magnitude at the northern boundary. Meanwhile the most frequent wind and its corresponding waves, and also circulation pattern in Lowe et al. [22] and [23] was studied to perceive the regional conditions. Here the two important boundary conditions which are waves and wind are expressed.

#### 7.3.1 Waves application

As it was mentioned before, the boundary of our computational domain in north was set on the reef flat. Setting the boundary in this position helped to give the effect of waves as velocity of the current over the reef. The model used to calculate velocity of the current is based on analytical model of waves driven current depth proposed by Hearn [16]. On a reef flat except in the total absence of incoming swell, oscillatory motions are dominated by surface gravity waves and bottom friction arises in the presence of waves. Referring to the waves friction Law in Hearn [16], background friction speed $u_f$
7.3. BOUNDARY CONDITIONS FOR SIMULATION

Figure 7.3: Historical waves and wind conditions recorded in Kaneohe bay during 2005-2006: a) significant waves height, b) peak waves direction, c) wind speed and d) wind direction all measured and recorded on Mokapu Peninsula, with the courtesy of Lowe et al. [22].

can be described by rotational speed of propagating waves.

\[ u_f = u_0^f \beta \left( \frac{h_r}{h_s} \right) (1 - \Gamma_s) + \Gamma_s \]  

(7.1)

In which

\[ u_0^f \equiv \pi H_0 / T, \quad \beta \equiv \gamma_r \gamma_b / \gamma_s^2, \quad h_s \equiv H_0 / \mu, \quad \mu \equiv \gamma_s^2 / \gamma_b, \quad \Gamma_s = 1 / [1 + (8/3 \gamma_s^2)] \]  

(7.2)

Where \( H_0 \) is incident waves height, \( T \) waves period, \( h_r \) depth of the reef, \( \gamma_r \) and \( \gamma_b \) and \( \gamma_s \) are the wave-breaking ratio at reef flat, wave breaking region and bulk of surf zone respectively. The numerical values were obtained from table 7.1 by Hearn [16]. The friction law does not contain turbulence related to wave breaking and this assumption is correct under the hypothesis that breaking is limited to the fore reef. Finally the current velocity over the reef can be written as below.

\[ u_r = (u_0^2 / \beta u_0^f) F_1(h_r / h_s) f_1(r) \]  

(7.3)

Here

\[ u_0^2 = \frac{g \Gamma_s h_r^2}{4 C_r a (1 - \Gamma_r)}, \quad F_1(h_r / h_b) = \frac{4 (h_r / h_s) [1 - h_r / h_s]}{\Gamma_s + (1 - \Gamma_s) h_r / h_s}, \]  

(7.4)

and

\[ f_1(r) = (1 + r + 1/3 r^2) / (1 + r), \quad r = (\Gamma_s / h_r) (h_s - h_r), \]  

(7.5)
(a) Bathymetry contour up to 5 meter and inflow position.

(b) Analytical velocity magnitude from eq.7.3 compared to interpolated data produced by Jia et al. [18].

Figure 7.4: Inflow position and velocity magnitude of that.

In which $a$ is distance from front to back of the reef flat, $C_f$ friction drag coefficient on the reef flat and $g$ is gravitational constant (acceleration). These parameters were also obtained from table 7.2 by Hearn [16]. Finally using the parameters and constants for Kaneohe bay given by Hearn [16], we can say that the current velocity over the reef flat is a function of incident wave height, wave period and also depth of the reef flat, i.e. $u_r = f(H_0, T, h_r)$.

In order to recognize the position of incoming and outgoing flow for our oceanic boundary line, time average of net currents vector from Lowe et al. [22] was regarded as reference. Based on this observation, position of incoming current over the reef was determined. Thereafter, northing and easting velocities were interpolated from the Oahu regional model data by Jia et al. [18] for our grid. The velocity magnitude $|u| = \sqrt{u^2 + w^2}$ (in which $w$ is northing velocity) was calculated, averaged in time and plotted. Then for specified inflow region, $u_r$ was calculated for different reef flat depths, different incident wave heights and time periods.
Looking at historical wind and wave directions measured during 2005-2006 in Kaneohe bay by Lowe et al. [22], the most frequent incident waves height is in the range of 1.5 to 2 m with an angle around 75° from north, which is correspondent to the wind speed around 5 m/s at the same direction of waves (histogram of waves and wind shown in fig. 7.3). Considering these, we observed that analytical current velocity over the reef matched with interpolated velocity from the data by Jia et al. [18] for $H_0 = 1.7$ m and $T = 9$ sec, for the range of $h_r$ from 1.6 to 2.6 m. Figure 7.4a shows the bathymetry contour and the position of inflow, and fig. 7.4b shows the analytical velocity magnitude of current over the reef compared to the interpolated values from Jia et al. [18].

The incoming current for our simulation was based on these analytical values, and the outgoing current was calculated in such a way to conserve mass of flow in the domain. At the moment we run the simulation for a fixed incoming and outgoing flows. The incoming flow is given as two components ($u$ and $w$) of the velocity magnitude in 75° from north.

### 7.3.2 Wind application

The wind boundary condition can be used by wind stress imposed on the water surface. This approach is based on the formula proposed by Wu [44]. The wind is applied 10 m above the sea surface, and the wind velocity has two horizontal components, and shear velocities at the surface can be calculated as below.

$$u_{r,i} = U_{10,i} \sqrt{C_{10,\rho_a/\rho_0}}$$

(7.6)

In which $U_{10,i}$ is the $i$ component of the wind speed 10 m above the water surface, $\rho_a$ is density of air, and $C_{10}$ (the drag coefficient) is computed as:

$$C_{10} = (0.8 + 0.065U_{10,i})10^{-3}.$$  

(7.7)

<table>
<thead>
<tr>
<th>Region</th>
<th>Wave breaking ratio</th>
<th>Setup coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Notation</td>
<td>Value</td>
</tr>
<tr>
<td>Wave breaking</td>
<td>$\gamma_b$</td>
<td>0.8</td>
</tr>
<tr>
<td>Reef flat</td>
<td>$\gamma_r$</td>
<td>0.5</td>
</tr>
<tr>
<td>Bulk of surf zone</td>
<td>$\mu, \gamma_s$</td>
<td>0.53, 0.67</td>
</tr>
</tbody>
</table>

Table 7.1: Numerical values related to wave-breaking and waves set-up by Hearn [16].
The induced stress at the sea surface can also be written as:

\[ \tau_i = \rho C_{10} U_{10,i}^2. \]  \hspace{1cm} (7.8)

Also a zero mean random fluctuation with 20% variance is added to the reference \( \tau \) in order to have more realistic forcing. The wind velocity 5 m/s in the direction of 75° from north is considered for this simulation since it was most frequent based on histogram showed in fig. 7.3 reproduced by Lowe et al. [22].

### 7.3.3 Solid boundaries

The solid boundaries in our simulation are related to the coastline and bathymetry. These were created by GID software and a triangular surface mesh was generated, finally these bodies were treated as immersed boundaries. The base of immersed boundary methodology already discussed in details in chapter 4, section 4.2. For this simulation we considered the solid boundary as rough surface.

To determine roughness height of the reef, logarithmic law of the velocity in turbulent bottom boundary layer was used based on the fact that in a fully developed turbulent boundary layer, velocity profile follows the logarithmic law and the mean velocity is related to turbulence generation by bed shear stress [29]. The law of the wall to relate the velocity to roughness and displacement height is:

\[ U(y) = \frac{\tau}{k} \ln \left( \frac{y - d}{y_0} \right). \]  \hspace{1cm} (7.9)

In which \( k = 0.41 \) is Von Karman constant, \( d \) is the displacement height and \( y_0 \) is the reef roughness length scale that is going to be used in our simulation. This approach is from Reidenbach et al. [29] who applied this formulae to find roughness length scale of a fringing reef in the Gulf of Aqaba.

We tried the displacement height (\( d \)) and roughness length scale (\( y_0 \)) in a wide range and minimized the error which was the difference between \( U(y) \) and log profile \( \ln(y) \) in

| Incident waves Friction Distance across Friction Drag |
|-------------------------|------------------|------------|-----------|
| height \( H_0 \) (m)    | Law              | Distance   | Coefficient \( C_r \) |
| 3.0                     | Wave             | 1500       | 0.1       |
| 1.5                     | Wave             | 1500       | 0.03      |
least square sense, finally we obtained roughness length scale $y_0 = 8.7 \text{ cm}$ for the reef flat. Reidenbach et al. [29] showed that the global roughness of the coral reef is one order of magnitude larger than the global roughness of sand, hence we considered the roughness height $y_0 = 0.87 \text{ cm}$ in the other regions.

7.3.4 Coastal model description

The simulation was carried out using LES – COAST, based on the explanations in chapter 2. The model is a high resolution LES solving three dimensional (top-hat) filtered Navier-Stokes equations (2.1), (2.2) and (2.3). In this simulation we did not consider stratification and salinity. Latitude of Kaneohe bay is $21.4^\circ$, therefore Coriolis force has an important effect on the flow.

The filtering is based on the cell size, therefore scales less than the cell sizes are modelled and larger scales are resolved. In coastal modelling, since horizontal length scale is much larger than the vertical length scale, two different eddy viscosity models are applied in horizontal and vertical. This is called two eddy viscosity anisotropic Smagorinsky model (ASM) developed by Roman et al. [32]. These two eddy viscosities are defined as below.

$$\nu_{t,h} = (C_h L_h)^2 |\mathbf{S}_h|, \quad (7.10)$$

$$\nu_{t,v} = (C_v L_v)^2 |\mathbf{S}_v|. \quad (7.11)$$

The horizontal length scale is defined as $L_h = \sqrt{\Delta x^2 + \Delta z^2}$, and the vertical length scale is equal to $L_v = \Delta y$. The empirical horizontal and vertical coefficients $C_h, C_v$ are obtained from fig. 7.5 reproduced by Roman et al. [32]. For our grid resolution
CHAPTER 7. APPLYING LES ON SEA WATER CIRCULATION IN KANEHOHE BAY

(a) Horizontal velocity magnitude contour and stream-traces.

(b) Vertical velocity contour.

Figure 7.6: Instantaneous flow field observation at 1 meter depth.

$C_h = 0.0125$ and $C_v = 0.345$ are considered. Two components of strain rate tensors are specified as below:

$$|S_h| = \sqrt{2S_{11}^2 + 2S_{33}^2 + 2S_{13}^2},$$

$$|S_v| = \sqrt{2S_{12}^2 + 2S_{22}^2 + 2S_{23}^2}.$$  \hspace{1cm} (7.12)

This is the only difference of coastal model with what was explained in chapter 2. Since the Reynolds numbers of oceanic flows are high, it is impractical to resolve near wall region, and wall layer model is employed (chapter 4 section 4.2). In the next section results of the simulation for instantaneous field are displayed.

7.4 Instantaneous flow field observations

Simulation was carried out with and a fixed Courant number equal to 0.5, using the settings mentioned above. After reaching a statistical steady state, instantaneous flow field observations are discussed in this section. Fig. 7.6 shows instantaneous flow field
7.4. **INSTANTANEOUS FLOW FIELD OBSERVATIONS**

at one meter depth. Most part of flow moves in wind direction, but there are some circulations according to fig. 7.6a.

![Figure 7.7: Instantaneous flow field observation at 3 meter depth.](image)

(a) Horizontal velocity magnitude contour and stream-traces.

![Figure 7.8: Instantaneous contour of the magnitude of horizontal velocity and stream-traces 6 m below the water surface.](image)

(b) Vertical velocity contour.

The main horizontal circulation is related to the west side of the bay. The incoming current from north is affected by a stronger flow passing over the reef from east to west,
and changes direction toward west. In the western side of the reef, the water exchanges to the lagoon and also Ship channel. Current in Ship channel has a different direction than the one passing over the reef since the flow goes out through Ship channel.

The flow in western side of the bay also changes direction toward south-west because of the coastline shape. The difference in the direction and also intensity of the flow makes the big circulation in western side of the bay.

A strong current is observed near the coastline in eastern side of the bay, since the wind is parallel to the coastline here, while going a bit farther from the coastline current strength decreases. This difference can lead to circulation in deeper level.

The flow over the reef has maximum horizontal velocity as it was expected from Lowe et al. [22]. Despite of this relative strong shallow water net current, the flow at the backside of lagoon does not include strong current. These current strength differences make some circulations at the deeper level.

Instantaneous vertical velocity at one meter depth (fig. 7.6b) displays an upward flow in eastern side of reef and downward flow in western side of that, showing that the flow follows a vertical rolling. The flow direction is downwind at the free surface. The wind ward sides of the coastline also illustrate downward flow while the leeward sides display upward flow.

Going deeper to three meters below water surface, another main horizontal circulation appears in eastern side of the bay. Flow in shallow water specially near the coastline is upwind, while in deeper regions the flow still follows wind direction. The flow is downward in windward parts of the coastline and upward in leeward sides of it. Many red and blue spots in fig. 7.7b indicate plenty of small up-welling and down-welling rolling structures are located next to each other.

Figure 7.8 shows instantaneous flow field six meter below the water surface. At this depth the flow direction in most of the regions is upwind. This reverse direction with respect to the free surface was expected due to the wind stress and vertical rolling of the flow. The main horizontal circulation at this depth is observed in eastern side of the bay.

In order to understand the flow field better in three dimensions, some cross-shore slices are shown in fig. 7.9. Zero values are blanked and depth of the domain is exaggerated with respect to horizontal length to visualize the flow better. Streamtraces in this figure show up-welling and down-welling of flow due to the strong net current differences.

Considering the contour of along-shore velocity $u$, negative values near water surface in most of the regions showing the flow goes toward west. Also there is a deviation
toward north near water surface. These two features reflect the effect of Coriolis force and wind stress on water surface, while in the bottom the along-shore velocity contour shows positive values in most of the regions meaning that the flow direction is opposite of wind direction due to vertical rolling.

Some along-shore slices in fig. 7.10 illustrates downwind direction of flow in water surface. The flow direction changes near the sea bed because of the vertical rolling. The presence of the rotational flows corresponds with the elongated structures shown in fig. 7.9.

7.5 Turbulence statistics

In this section, temporal averaged quantities in 24 hours of simulation time are illustrated. Figure 7.11a shows temporal averaged horizontal velocity contour and stream-tracers one meter below the water surface. In west side of the bay a large circulation is seen, and in other regions the small circulations which were observed in instantaneous field shrank. The deviation of flow toward north-west can be clearly observed over the reef because of the Coriolis force.

Looking at the averaged vertical velocity contour at a depth of one meter (fig. 7.11b), the flow direction is downward at upwind sides of the reef (east of reef) and coastline, and it is upward at the leeward sides of the coastline and also the reef(west of reef). Comparing the averaged vertical velocity with the instantaneous one (fig. 7.6b), a more homogeneous field is illustrated since the very small blue and red colors transforms to bigger spots, meaning that very small vertical vortices disappeared.

Going deeper at a depth of three meters, in addition to the western anti-cyclonic circulation, another circulation appears in eastern side of the bay. This circulation can be due to the net current difference which is stronger in south-east. Mean vertical velocity contour shows more mixing than the lower depth in fig. 7.12b.

At six meters depth the flow is in opposite direction of the wind almost everywhere. The circulation in western side of the bay vanishes, and eastern anti-cyclonic circulation moves to south-east. Mean along-shore velocity contour $u$ and stream-lines in different slices in fig. 7.14 show that small vertical rolling structures have disappeared, and instead of that bigger vortices are observed, as we expected this from mean vertical velocity contour compared with instantaneous plot.

Small rolling structures vanish averaging the quantities in time and larger vortices are observed. The velocity direction at the water surface and sea bed can be the same or opposite each other as it can be seen from cross-shore slices (fig. 7.14) since there
are counter-rotating vortices.

Figure 7.14a shows that the water flows out from the bay through Ship channel. While the flow direction is toward west near the channel, a reverse direction is observed at water surface in the southern part. Also the same situation can be seen in Sampan channel (fig. 7.14e). These are in correspondence to the horizontal circulations.

Zooming in the reef in fig. 7.16a on a cross-shore slice, shows that the incoming current from the north, and then is affected by strong current over the reef which is deviated toward north because of Coriolis force. Inside the lagoon the flow close to the water surface comes upward while a bit deeper the flow is downward. This flow motion makes an anti-clockwise vertical rolling near the reef and a clock-wise rolling far from the reef.

Finally the flow direction a bit farther from the reef is toward south. From a along-shore slice (fig. 7.16b) it can be displayed that the flow near water surface is upward in east side of the reef, and downward a bit deeper. The flow near the water surface in the same direction of the wind from east to west, and counter rotating circulations occur in deeper level.

Despite of the reverse flow direction on water surface in cross-shore slices inside the channels, along-shore slices in fig. 7.15 show that the wind is dominant at the water surface, and the flow is toward west. Also on the sea bed the flow direction is in opposite with the flow direction on the water surface.

Counter-rotating eddies which are evidenced in cross-sectional areas are not generated by Stokes drift since it is not considered in the simulation. They are generated by free surface stresses giving rise to turbulent large scale sub surface coherent structures aligned in the surface stress direction (they are not shown here), which are common in wall bounded or interface turbulent flows. These vertical eddies contribute to vertical Reynolds stress generation which are responsible for vertical mixing. The vertical eddy viscosity can be quantified as in Coleman et al. [9].

\[
\nu_v = \sqrt{\langle u'v' \rangle^2 + \langle w'v' \rangle^2} + \nu_{t,v} \tag{7.14}
\]

And the horizontal eddy viscosity also can be written as below.

\[
\nu_h = \sqrt{\langle u'w' \rangle^2 + \langle v'w' \rangle^2} + \nu_{t,h} \tag{7.15}
\]

In which we sum the values obtained from resolved part and sub-grid scale part; \(\nu_{t,v}\) and \(\nu_{t,h}\) are obtained from equations (7.11) and (7.10) respectively. Figures 7.17
and 7.18 display the variation of vertical and horizontal eddy viscosities at different depths respectively.

Figures 7.17a and 7.18a illustrate variation of vertical and horizontal eddy viscosities at one meter depth. At this depth the vertical eddy viscosity in south-west of the reef is maximum while the horizontal eddy viscosity is larger in lagoon. Also the horizontal eddy viscosity is three order of magnitude bigger than the vertical eddy viscosity.

At three meters depth the vertical eddy viscosity experiences more changes than the one at one meter depth, while the horizontal eddy viscosity does not display too much difference. A deeper view six meters below the water surface also shows an increase in the vertical eddy viscosity, while a decline in the variations of the horizontal eddy viscosity is observed (fig. 7.18c).

Near the sea bottom at 10 meters depth, still the vertical eddy viscosity illustrating high values (fig. 7.17d), while the horizontal eddy viscosity displays a decline according to fig. 7.18d. The vertical and horizontal eddy viscosities are also illustrated in along-shore and also cross-shore slices to have a three dimensional visualization.

Some cross-shore slices show that the vertical eddy viscosity is maximum at deeper levels, and mostly in lagoon while the horizontal eddy viscosity is large at a comparatively lower depth, and not only in lagoon but also near the channels( figs. 7.19 and 7.20). The along-shore slices reveal that in the north of the bay the values for the vertical and horizontal eddy viscosities decrease (figs. 7.21 and 7.22).

Turbulent kinetic energy (TKE) is also analysed to identify the distribution of turbulence intensity along the depth. Figure 7.23 shows the variation turbulent kinetic energy at four different depths. This quantity is calculated from the formula below.

\[
TKE = \frac{1}{2}(u'^2 + v'^2 + w'^2)
\]

The turbulent kinetic energy is non-dimensionalized by square of the shear velocity at the water surface, obtained from the wind stress at the free surface; \( u_r = \sqrt{u_{r,x}^2 + u_{r,z}^2} \). TKE at one meter depth has the larger values between the lagoon and its connection to the channels, also in eastern side of the bay. Thereafter, three meters below the water surface this energy decreases specially in western side of the bay, and finally at the depth of ten meters this quantity has its highest value in the lagoon.

Some cross-shore slices in fig. 7.24 display the large values of TKE are in the south part of the bay, in lagoon, and also where water exchanges between the lagoon and the channels. Along-shore slices also show the maximum values mostly in the south of the reef, and the connection between the lagoon and the channels (fig. 7.25).
7.6 Conclusion

In this chapter we show the application of LES – COAST to the analysis of a coral reef bay. The model is suitable to analyse water circulation in ports or lakes. This model is three dimensional and unsteady. Turbulent mixing is accomplished using large eddy simulation with two-eddy viscosity Smagorinsky model. Complex geometries such as bathymetry and coastline are treated as immersed boundaries.

Wind was applied on the water surface all around the bay. Analytical model proposed by Hearn [16] was used to calculate the velocity of current resulting from waves over the reef, and it was set as boundary condition. The velocity of current over the reef was interpolated from Oahu regional model by Jia et al. [18] at the boundary of our grid. Thereafter to calculate analytical current velocity based on the model proposed by Hearn [16], the analytical current velocity computed from a most frequent waves height $H_0 = 1.7 \text{ m}$ with time periodic of $T = 9 \text{ sec}$ given from Lowe et al. [22] matched the interpolated values for a range of the reef depth $h_r$ from 1.6 to 2.6 m. Since the time step of our simulation was close the time period of the waves, no oscillation applied at the inflow.

The inflow and outflow regions were located based on the currents showed by Lowe et al. [22], and the outflow was in such a way to conserve mass in the domain. Finally the LES model was applied on Kaneohe bay in high resolution in order to analyse water circulation in different areas.

Small vortices which were visible in instantaneous observations disappeared when temporal averaging was carried out, and main circulations remained. Cross-shore slices revealed that counter-rotating vertical circulations occur even close to water surface while in along-shore slices these counter-rotating circulations happen in deeper levels.

Strong current was observed over the reef while the currents in the lagoon were much weaker. High rate of vertical mixing was illustrated in lagoon specially moving in the deeper levels while horizontal mixing was maximum closer to the water surface. The TKE distribution showed a relatively higher intensity in the east and west parts of lagoon.

Average residence time gives the idea of the time required that the water of a specified coastal zone is replaced. This information is very useful for pollution dispersion and also marine biology. The capacity of a coastal zone to hold water divided by the rate of incoming or outgoing current can roughly give the residence time of that coastal region. A map of residence time of Kaneohe bay illustrates a high degree of spatial heterogeneity, as it was mentioned and expected from Lowe et al. [22].
7.6. CONCLUSION

The largest average residence time is related to the eastern side of the bay, zone 6 in fig. 7.26 which is 10.2 days. Thereafter the water takes 7 days to be replaced in the lagoon (zone 5). Western part of the bay has residence time of 4.7 days which is displayed as zone 4. Finally the average residence times of zones 3, 1 and 2 are 1.7, 1.5 and 1 days respectively.

The values we obtained are different from Lowe et al. [22], specially for zone 6 which in their numerical model has the residence time at least three weeks. This difference can be due to the different approaches followed to obtain this quantity since they evaluated the residence time by conducting a series of numerical experiments using Lagrangian particle tracking. In their studies also zones 6 and 5 had the largest residence time, while the smallest value was related to zone 1 which for our case was zone 2. This can be because of the constant current we considered over the reef as inflow.
Figure 7.9: Contour plots of instantaneous along-shore velocity $u$ with instantaneous stream traces at five different positions specified by red line.
Figure 7.10: Contour plots of instantaneous cross-shore velocity $w$ with instantaneous streamlines in six different positions, specified by red line.
(a) Horizontal velocity magnitude contour and stream-traces.

(b) Vertical velocity contour.

Figure 7.11: Temporal averaged flow field observation at 1 meter depth.
7.6. CONCLUSION

(a) Horizontal velocity magnitude contour and stream-traces.

(b) Vertical velocity contour.

Figure 7.12: Temporal averaged flow field observation at 3 meter depth.

Figure 7.13: Temporal averaged contour of the magnitude of horizontal velocity and streamtraces 6 m below the water surface.
Figure 7.14: Contour plots of temporal averaged along-shore velocity $u$ with stream traces at five different positions specified by red line.
Figure 7.15: Contour plots of temporal averaged cross-shore velocity $w$ with streamlines in six different positions, specified by red line.
(a) Averaged along-shore velocity $u$ contour and stream-line on a cross-shore slice.

(b) Averaged cross-shore velocity $w$ contour and stream-traces on an along-shore slice.

Figure 7.16: A close-up to the reef in cross-shore and along-shore slices.
7.6. CONCLUSION

(a) At 1 meter depth.

(b) At 3 meters depth.

(c) At 6 meters depth.

(d) At 10 meters depth.

Figure 7.17: Contour plots of vertical and horizontal eddy viscosities at different depths.
(a) At 1 meter depth.

(b) At 3 meters depth.

(c) At 6 meters depth.

(d) At 10 meters depth.

Figure 7.18: Contour plots of horizontal eddy viscosity at different depths.
Figure 7.19: Vertical eddy viscosity contour in four different cross-shore slices.

Figure 7.20: Horizontal eddy viscosity contour in four different cross-shore slices.
Figure 7.21: Vertical eddy viscosity contour in four different along-shore slices.

Figure 7.22: Horizontal eddy viscosity contour in four different along-shore slices.
7.6. CONCLUSION

(a) 1 m below the water surface.

(b) 3 m below the water surface.

(c) 6 m below the water surface.

(d) 10 m below the water surface.

Figure 7.23: Contour plots of turbulent kinetic energy at four different depths.
Figure 7.24: Vertical eddy viscosity contour in four different cross-shore slices.
7.6. CONCLUSION

Figure 7.25: Horizontal eddy viscosity contour in four different along-shore slices.

Figure 7.26: Specified domains for calculating average residence time.
Bibliography


