RESIDUAL-BASED TURBULENCE MODELS FOR INCOMPRESSIBLE FLOWS IN DOMAINS WITH MOVING BOUNDARIES

BY

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DISSERTATION

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Abstract

This dissertation presents residual-based turbulence models for problems with moving boundaries and interfaces. The method is derived employing the Variational Multiscale (VMS) framework, which gives rise to several modeling options that are exploited to obtain accurate turbulence models. To accommodate problems with moving boundaries such as fluid-structure interaction and free-surface problems, the formulation is cast in an Arbitrary Lagrangian-Eulerian (ALE) frame of reference.

Multiple models of increasing degree of mathematical and algorithmic sophistication are presented. In all the cases, we assume a multiscale decomposition of the solution fields into overlapping components of different scale. The scales that can be accurately captured by the finite element discretization are numerically resolved, and are termed as the coarse scales, while the sub-grid scales, which may not be accurately represented by the finite element discretization, are termed as the fine-scales. The key idea of the VMS framework is to derive models for the fine scales in terms of the coarse scales, and then variationally project the fine-scale models onto coarse-scale space. This approach results in formulations that only depend on the coarse scales, while the effects of the fine scales on the coarse-scale fields are fully accounted for via the additional terms that arise due to the multiscale decomposition of the solution fields. In this dissertation, the fine scales are modeled using a bubble functions approach. This enables the fine-scale problem to be solved on elements or patches of elements. As a consequence, the presented algorithms are amenable for parallel implementation. The simplest fine-scale model presented here is derived introducing up-winding ideas to the discrete problem that governs the fine scales. To derive expressions for more sophisticated fine-scale models, VMS ideas are also applied to the fine-scale sub-problem.

A significant feature of the bubble functions approach adopted here is that the derived turbulence models are free of any embedded or tunable parameters. Another significant feature of the method is that it is mathematically consistent because the fine-scale models are driven by the residual of the Euler-Lagrange equations for the coarse scales. Consequently, when the coarse scales are able to represent the exact solution of the problem, the fine-scale models vanish.
Numerical attributes of the developed models are investigated via an exhaustive set of numerical tests. One of the classes of problems investigated has fix boundaries while the other has moving boundaries. The results are compared to reference experimental and numerical results, and excellent agreements are observed.
To Gemma
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Chapter 1

Introduction

1.1 Motivation

In the last few decades the use of Computational Fluid Dynamics (CFD) to study fluid dynamics problems has grown significantly. This increase is a consequence of the exponential growth of available computational resources, which has enabled the study of problems with increasingly higher number of degrees of freedom. At the same time that the computing power has increased, the efficiency of numerical algorithms employed to solve fluid problems has also improved. Therefore, the computational cost of solving a given problem has decreased as a consequence of the improvement of the numerical algorithms. These two advances are starting to make CFD techniques a feasible tool for studying fluid flows in industrial-strength problems.

A significant number of fluid dynamics problems of engineering interest involve moving boundaries. The two most paradigmatic cases are fluid-structure interaction and free surface flow problems. In addition, some of these problems have domains with very complex boundaries. The main objective of the present dissertation is to develop parameter-free turbulence models for problems with moving boundaries. The formulations are derived for unstructured meshes, which are very suited to discretize problems with complex boundaries. So, the proposed formulations, which accommodate $h$- and $p$-refinements, are ideally suited to study industrial-strength problems.

A direct technique to solve turbulent flows is the Direct Numerical Simulation (DNS) approach, in which all the scales involved in the flow are numerically resolved [103, 134]. Due to the disparity of length and temporal scales present in turbulent flows, this approach requires discretizations that are very fine, and thus, the computational cost of DNS is extremely high. In most industrial-strength problems the cost of DNS is prohibitive. On the other hand, Reynolds Averaged Navier-Stokes (RANS) techniques only resolve the largest scales involved in the fluid flow [119] and therefore, it is less computationally intensive than
DNS. However, only the averaged features of the flow are obtained. The Large Eddy Simulation (LES) approach [118, 81, 44, 29, 68, 102, 85] is a technique that lies between DNS and RANS. It takes advantage of the fact that the smallest scales of turbulent flows are isotropic and are considered to have a universal behavior. In LES, these isotropic scales are modeled, while the larger scales are resolved numerically. This approach yields algorithms that are more accurate than RANS models but less computationally intensive than DNS.

The Variational Multiscale (VMS) framework follows the philosophy of LES techniques, as it models the effects of the smallest scales of the flow and numerically resolves the largest scales. The VMS framework was proposed by Hughes [64] as a method to derive stabilized mixed-field formulations for the Navier-Stokes equations, and was later extended to turbulence modeling [65, 66, 67, 26, 106]. It assumes an overlapping multiscale decomposition of the solution fields in coarse or resolvable scales, and fine or sub-grid scales. The key idea of the approach is the modeling of the problem that governs the fines scales. This fine scale model, which is generally driven by the residual of the Euler-Lagrange equations for the coarse scales, is variationally embedded in the coarse scale problem. Since the fine-scale models only depend on the coarse-scale fields, the resulting formulations are expressed solely in terms of the coarse scale, but the effects of the fine scales are accounted for via the embedded fine-scale models. For recent advances in the VMS framework see for example [78, 47, 35, 10, 25, 2, 11, 43, 55] and references therein.

The present dissertation derives turbulence models for the incompressible Navier-Stokes equations using the VMS framework. The most important contribution of this dissertation to the VMS framework is the approach adopted to model the fine scales. The fine-scale models are derived employing a bubble function approach that localizes the domain of the fine-scale problems to element interiors. As a result, the proposed models are amenable for implementation in scalable codes. In addition, the resulting formulations do not possess any embedded or tunable parameter, and as a consequence, the developed computer codes are easy to use.

To accommodate problems with moving boundaries, VMS formulations need to be complemented by a technique that represents the location of the evolving boundaries. In the literature, these methods are classified as interface-capturing and interface-tracking techniques. In interface-capturing techniques, the moving boundaries are defined by a scalar
field, and the fluid equations are solved employing a fix mesh. Some methods that fall in this category are the Volume of Fluids techniques [54, 31, 84, 82], in which the scalar field represents the fraction of fluid in the mesh elements, and the Level Set techniques [120, 3], in which the scalar field represents the distance of each point to the free surface. The advantage of using an interface-capturing technique is that the computational mesh does not deform, and as a consequence, the aspect ratio of the elements is conserved independently of the evolution of the boundaries. Therefore, re-meshing is not needed in any case. On the other hand, in interface-tracking approaches, the mesh in which the fluid equations are solved deforms to adapt to the evolving boundaries. In these approaches, the locations of the nodes that are on the moving boundaries track the displacement of the boundaries. The methods that are based on an Arbitrary Lagrangian-Eulerian (ALE) frame of reference [57, 56] fall in the category of interface-tracking approaches. In ALE formulations, the locations of the nodes that do not lay on the boundaries are updated at every time step to attempt to maintain the aspect ratio of the elements. For problems in which the boundaries undergo very large deformations, the elements aspect ratio may deteriorate, and re-meshing is sometimes needed. Another interface-tracking technique is the Particle Finite Element Method (PFEM) [110, 28], which solves the fluid equations using a Lagrangian description. This approach does not require a computational mesh, and as a consequence, circumvents the mesh distortion issues. However, a tessellation needs to be computed at every time step to perform the computations, and therefore, the computational cost of particles methods can be substantial. Space-time methods [124, 125] are another type of interface-tracking techniques. The space-time domain evolves in the time coordinate axes to adapt to the moving boundaries. Space-time techniques have the same limitations as ALE-based techniques.

The presented VMS formulations are cast in an ALE frame of reference to accommodate domains with moving boundaries. We adopt an ALE approach because of its accuracy. A common situation in which the accuracy of the ALE based methods is clearly manifested is found on the study of boundary layers that are attached to a moving boundary. Near the moving boundaries, very fine elements need to be employed. In ALE approaches, as the domain boundaries move, the distribution of element sizes is approximately maintained. Consequently, near the deformed boundaries, the mesh resolution is conserved, and therefore
the boundary layer can be accurately captured independently of the displacement of the domain boundaries.

1.2 Dissertation outline

The objectives of the present dissertation are achieved by successive refinements of VMS-based models. The first model presented is derived in Chapter 2, and one layer of sophistication is added in every subsequent Chapter. The remaining part of the dissertation is organized as follows:

- In Chapter 2, a variational method for incompressible laminar flows is presented. The method is developed assuming a multiscale decomposition of the velocity field in coarse and fine-scale components. A model for the fine-scales is derived employing a bubble functions approach that introduces up-winding effects to the problem that governs the fine-scales. The convergence and accuracy of the proposed method is shown via a series of numerical tests.

- In Chapter 3, the formulation proposed in Chapter 2 is cast in an Arbitrary Lagrangian-Eulerian frame of reference to accommodate problems with moving boundaries. Numerical tests show the robustness of the mesh moving scheme employed and the accuracy of the formulation.

- In Chapter 4, we extend the formulation presented in Chapter 2 for laminar flows to turbulence flows by relaxing some of the assumptions that are done in Chapter 2. The derivation of the fine-scale model gives rise to various modeling options that are numerically investigated by studying turbulent flows in a channel with parallel walls. A study of a turbulent flow around a circular cylinder shows the applicability of the formulation to more complex problems.

- In Chapter 5, the turbulence models developed in Chapter 4 are refined to accurately model problems that are discretized with unstructured tetrahedral meshes. The solution fields are decomposed in three hierarchical components of different scale. The finest scales are used to stabilize the mixed field problem that governs the intermediate scales. The intermediate scales provide stability to the problem that governs the coarsest scales. In addition, they also serve as a turbulence model. The coarse scales represent the resolvable scales of the flow. A
study of turbulent channel flows and the flow around an airfoil show the accuracy and applicability of the improved formulation.

- In Chapter 6, the formulation presented in Chapter 5 is expressed in an ALE frame of reference to extend the applicability of the formulation to problems with moving boundaries. The resulting turbulence model is applied to study a plunging airfoil.

- In Chapter 7, the method presented in Chapter 6 is employed to study two turbulent open channel flow problems. While the first one has a flat bottom surface, the bottom surface of the second one is undulated.

- In Chapter 8, a description of the approach used to implement the models derived in Chapters 2-7 is presented. In addition, a study of the performance of the developed parallel code is carried out.

- Conclusions are drawn in Chapter 9. The main contributions of the present dissertation to the field of turbulence modeling are remarked, and possible future research directions are outlined.
Chapter 2

A Variational Multiscale stabilized formulation for the incompressible Navier-Stokes equations*

2.1 Motivation

Stabilized methods now enjoy a strong presence in the field of computational fluid dynamics (CFD). These methods were developed to address the shortcomings of the classical Galerkin method when applied to advection dominated flows and mixed field problems where arbitrary combinations of interpolation functions for the pressure and velocity fields invariably yield unstable discretized formulations [88]. A significant step toward the development of stabilized methods was the Streamline Upwind/Petrov-Galerkin (SUPG) method by Hughes and colleagues [19, 58]. SUPG eventually led to the development of the Galerkin/Least-Squares (GLS) stabilization methods [59, 63, 36, 37, 52, 86, 69]. In the context of advection dominated phenomenon, a fundamental contribution of these methods was the stabilization of the advection operator without upsetting consistency or compromising accuracy, and circumvention of the Babuska-Brezzi (inf-sup) condition. The foundations of these methods were made precise in mid 90's when Hughes presented the Variational Multiscale (VMS) method [64, 65]. Stabilized methods have also enjoyed from the developments in the residual-free bubble methods by Brezzi and co-workers [15, 6, 16, 17, 18] and the unusual stabilized methods by Franca and co-workers [38, 39]. Stabilized methods were extended to space-time finite element techniques by Tezduyar and co-workers [124, 125, 126] and Masud and Hughes [86]. A good chronological account of stabilized methods is provided in [88]. For recent advances in stabilized methods, see for example [41, 108, 40, 33, 128, 22, 24, 46, 89, 30, 92, 129] and references therein.

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This Chapter is an extension of the earlier works on advection dominated flows performed by Masud and co-workers [89, 92]. In [92] we had employed fixed point iteration idea to linearize the coarse and fine scale sub-problems that arise in the Variational Multiscale framework, and it lead to a stabilized method for the incompressible Navier-Stokes equations. In the current work we present a consistent linearization of the nonlinear coarse and fine scale sub-problems, and substitution of the fine scales extracted from the fine-scale problem into the coarse-scale variational form leads to the new stabilized method. The solution of the fine-scale or the sub-grid scale problem which is an integral component of the proposed procedure for developing stabilized methods automatically yields an explicit definition of the stabilization operator \( \tau \). Another significant contribution of the Chapter is a numerical technique for evaluating the advection part of the stabilization operator \( \tau \) that brings in the notion of up-winding in the resulting method.

An outline of the Chapter is as follows. In Sec. 2.2, we present the strong form and the classical weak form of the incompressible Navier-Stokes equations. Consistent linearization of the nonlinear equations performed in the Variational Multiscale setting leads to the new multiscale/stabilized formulation that is developed in Sec. 2.3. The structure of the stabilization tensor and a numerical scheme to evaluate its advection part are presented in Sec. 2.4. Section 2.5 presents a convergence study for a family of 3D tetrahedral and hexahedral elements. An extensive set of numerical simulations of lid-driven cavity flows for various Reynolds number are also presented. Conclusions are drawn in Sec. 2.6.

### 2.2 The incompressible Navier-Stokes equations

Let \( \Omega \subseteq \mathbb{R}^{n_{sd}} \) be an open bounded region with piecewise smooth boundary \( \Gamma \). The number of space dimensions, \( n_{sd} \) is equal to 3. The conservative form of the incompressible Navier-Stokes equations can be written as:

\[
\begin{align*}
\mathbf{v}_{,t} + \nabla \cdot (\mathbf{v} \otimes \mathbf{v}) - 2\nu \nabla \cdot \mathbf{e}(\mathbf{v}) + \nabla p &= \mathbf{f} & \text{in } \Omega \times ]0, T[ \quad (2.1) \\
\nabla \cdot \mathbf{v} &= 0 & \text{in } \Omega \times ]0, T[ \quad (2.2) \\
\mathbf{v} &= \mathbf{g} & \text{on } \Gamma_g \times ]0, T[ \quad (2.3) \\
\sigma \cdot \mathbf{n} &= (2\nu \mathbf{e}(\mathbf{v}) - pI) \cdot \mathbf{n} = \mathbf{h} & \text{on } \Gamma_h \times ]0, T[ \quad (2.4)
\end{align*}
\]
\[ \mathbf{v}(x,0) = \mathbf{v}_0 \quad \text{on } \Omega \times \{0\} \quad (2.5) \]

where \( \mathbf{v} \) is the velocity vector, \( p \) is the kinematic pressure, \( \mathbf{f} \) is the body force vector, \( \nu \) is the kinematic viscosity assumed positive and constant, \( \mathbf{I} \) is the identity tensor, \( (\cdot)_t \) represents time derivative, and \( \otimes \) denotes the tensor product (e.g., in indicial notation, \( [\mathbf{u} \otimes \mathbf{v}]_{ij} = u_i v_j \)). \( \mathbf{\varepsilon} \) is the strain rate tensor, which is defined as \( \mathbf{\varepsilon}(\mathbf{v}) = (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)/2 \).

Equations (2.1)-(2.5) represent balance of momentum, the continuity equation, the Dirichlet and Neumann boundary conditions, and the initial condition, respectively.

The advection term in equation (2.1), \( \nabla \cdot (\mathbf{v} \otimes \mathbf{v}) \), can be split into two parts:

\[ \nabla \cdot (\mathbf{v} \otimes \mathbf{v}) = \mathbf{v} \cdot \nabla \mathbf{v} + \beta (\nabla \cdot \mathbf{v}) \mathbf{v} \quad (2.6) \]

where parameter \( \beta \in [0,1] \). If \( \beta = 1 \), the discretized problem conserves momentum, if \( \beta = 0.5 \), the total energy of the discretized problem is conserved, and if \( \beta = 0 \), we recover the classical non-conservative form of the momentum equation [115].

### 2.2.1 The standard weak form

Let \( \mathbf{w} \) and \( q \) represent the weighting functions for velocity and pressure, respectively. The appropriate spaces of weighting functions for velocity and pressure are: \( \mathbf{w} \in \mathbf{V} = (H^1_0(\Omega))^d \) and \( p \in \mathbf{P} = C^0(\Omega) \cap L^2(\Omega) \). The appropriate spaces for the velocity and pressure trial solutions are the corresponding time-dependent spaces \( \mathbf{V}_t \) and \( \mathbf{P}_t \). The weak form of the problem is given as:

\[
\begin{align*}
(w, v_j) + (w, v \cdot \nabla v) + \beta (w, v \cdot \nabla v) \\
+ \left( \nabla' w, 2v \nabla' v \right) - \left( \nabla' w, \mathbf{f} \right) &= (w, \mathbf{f}) + (w, \mathbf{h})_{\Gamma _n} \\
(q, \nabla v) &= 0
\end{align*}
\quad (2.7, 2.8)
\]

where \( (, \cdot) = \int_{\Omega} (\cdot) \, d\Omega \) is the \( L_2(\Omega) \) - inner product.

**Remark:** Equations (2.7) and (2.8) present the standard weak form of the problem. It is well documented that within the framework of standard Galerkin methods, advection dominated flows lead to spurious oscillations in the pressure field. This issue is usually addressed with...
the help of SUPG and GLS type methods. However, in the following sections we will develop a modified formulation that is based on the idea of multiscale modeling and yields a new method that can effectively control spurious oscillations in advection dominated flows.

2.3 The Variational Multiscale method

The Variational Multiscale Method [64, 65, 95] is based on an additive decomposition of the response function into coarse and fine scales. The bounded domain $\Omega$ is considered discretized into non-overlapping sub-regions $\Omega^e$ (element domains) with boundaries $\Gamma^e$, $e=1, 2, \ldots, nel$. The union of element interiors and element boundaries is indicated as $\Omega'$ and $\Gamma'$, respectively:

$$\Omega' = \bigcup_{e=1}^{nel} (\text{int}) \Omega^e \quad \text{(element interiors)} \quad (2.9)$$

$$\Gamma' = \bigcup_{e=1}^{nel} \Gamma^e \quad \text{(element boundaries)} \quad (2.10)$$

We assume an overlapping sum decomposition of the velocity field into coarse or resolvable scales and fine or sub-grid scales. Fine scales can be viewed as the scales that are associated with the regions of high velocity gradients.

$$v(x,t) = v(x,t) + v'(x,t) \quad (2.11)$$

We assume that $v'$ is represented by piecewise polynomials of sufficiently high order, continuous in $x$ but discontinuous in time. In particular, $v'$ is assumed to be composed of piecewise constant-in-time functions leading to $v(x,t) = \bar{v}(x,t) + v'_c(x)$. Consequently, taking time derivative of $v(x,t)$ we get:

$$v'_c(x,t) = \bar{v}'(x,t) \quad (2.12)$$

Likewise, we assume an overlapping sum decomposition of the weighting function into coarse and fine scale components indicated as $\bar{w}$ and $w'$, respectively:

$$w(x) = \bar{w}(x) + w'(x) \quad (2.13)$$
We further make an assumption that the fine scales although non-zero within the elements, vanish identically over the element boundaries:

\[ \mathbf{v}_i' = \mathbf{w}' = \mathbf{0} \text{ on } \Gamma' \quad (2.14) \]

Consistency of the method requires that the spaces of functions for the coarse and fine scales are linearly independent. A comprehensive discussion on the topic is presented in [64, 65].

### 2.3.1 Multiscale decomposition of the variational problem

We substitute the trial solutions (2.11)-(2.12) and the weighting functions (2.13) in the standard variational form (2.7) and (2.8), and it yields the following set of equations:

\[
\begin{align*}
\langle \mathbf{w} + \mathbf{w}', \mathbf{v} \rangle &+ \langle \mathbf{w} + \mathbf{w}', (\mathbf{v} + \mathbf{v}') \cdot \nabla (\mathbf{v} + \mathbf{v}') \rangle \\
&+ \beta (\mathbf{w} + \mathbf{w}', (\mathbf{v} + \mathbf{v}') \cdot \nabla (\mathbf{v} + \mathbf{v}')) + (\nabla' (\mathbf{w} + \mathbf{w}'), 2v \nabla' (\mathbf{v} + \mathbf{v}')) \\
&- (\nabla \cdot (\mathbf{w} + \mathbf{w}'), p) = (\mathbf{w} + \mathbf{w}', \mathbf{f}) + (\mathbf{w} + \mathbf{w}', \mathbf{h})_{\text{}}_{\Gamma_0} \\
(q, \nabla \cdot (\mathbf{v} + \mathbf{v}')) &= 0 \quad (2.15)
\end{align*}
\]

The weak form of the momentum equations is nonlinear because of the skew convection term. However, it is linear with respect to the weighting function slot. Exploiting this linearity, we split (2.15) into two parts: the coarse-scale sub-problem and the fine-scale sub-problem. These sub-problems can be written in a residual form as follows:

**Coarse-scale sub-problem:**

\[
\begin{align*}
\mathcal{R}_1(\mathbf{w}_i; \mathbf{v}_i, p) &\overset{\text{def}}{=} (\mathbf{w}_i, \mathbf{v}_j) + (\mathbf{w}_i, (\mathbf{v} + \mathbf{v}') \cdot \nabla (\mathbf{v} + \mathbf{v}')) \\
&+ \beta (\mathbf{w}_i, (\mathbf{v} + \mathbf{v}') \cdot \nabla (\mathbf{v} + \mathbf{v}')) + (\nabla' \mathbf{w}_i, 2v \nabla' (\mathbf{v} + \mathbf{v}')) \\
&- (\nabla \cdot \mathbf{w}_i, p) - (\mathbf{w}_i, \mathbf{f}) - (\mathbf{w}_i, \mathbf{h})_{\Gamma_0} = 0 \quad (2.17)
\end{align*}
\]

**Fine-scale sub-problem:**

\[
\begin{align*}
\mathcal{R}_2(\mathbf{w}_i; \mathbf{v}_i, p) &\overset{\text{def}}{=} (\mathbf{w}_i, \mathbf{v}_j) + (\mathbf{w}_i, (\mathbf{v} + \mathbf{v}') \cdot \nabla (\mathbf{v} + \mathbf{v}')) \\
&+ \beta (\mathbf{w}_i, (\mathbf{v} + \mathbf{v}') \cdot \nabla (\mathbf{v} + \mathbf{v}')) + (\nabla' \mathbf{w}_i, 2v \nabla' (\mathbf{v} + \mathbf{v}')) \\
&- (\nabla \cdot \mathbf{w}_i, p) - (\mathbf{w}_i, \mathbf{f}) = 0 \quad (2.18)
\end{align*}
\]
The general idea at this point is to solve the fine-scale problem, defined over the sum of element interiors to obtain the fine scale solution. This solution is then substituted in the coarse-scale problem thereby eliminating the explicit appearance of the fine scales while still modeling their effects. Both coarse and fine scale equations are in fact nonlinear equations because of the convection term, and in order to solve them we need to linearize them. In this work we perform consistent linearization of the coarse and fine-scale sub-problems as described in the following sub-sections.

2.3.2 Solution of the fine-scale sub-problem

In the approach adopted here, we solve the fine scales in a direct nonlinear fashion. We take variational derivative of the nonlinear operator \( \mathcal{R}_3(\bullet,\bullet) \) to obtain the linearized operators \( \mathcal{L}(\mathcal{R}_3(\bullet,\bullet)) \) defined as follows:

\[
\mathcal{L}(\mathcal{R}_3(w';\bar{v},v',p)) \overset{\text{def}}{=} \left. \frac{d}{d\varepsilon} \mathcal{R}_3(w';\bar{v} + \varepsilon \partial v, v' + \varepsilon \partial v', p + \varepsilon \partial p) \right|_{\varepsilon=0} \quad (2.20)
\]

Applying (2.20) to (2.19), linearizing about the known solution \( \hat{v} \) and \( \hat{p} \), and ignoring the higher order terms, we get the linearized fine scale problem

\[
(w',\partial \bar{v}) + (w',(\delta \bar{v} + \delta v') \cdot \nabla \hat{v} + \hat{v} \cdot (\delta \bar{v} + \delta v'))
+ \beta (w',(\delta \bar{v} + \delta v') \nabla \cdot \hat{v} + \hat{v} \nabla \cdot (\delta \bar{v} + \delta v'))
+ (\nabla' w', 2v' \nabla (\delta \bar{v} + \delta v')) - (\nabla \cdot w', \delta \partial p) = -\mathcal{R}_3(w';\hat{v}, \hat{p}) \quad (2.21)
\]

where \( \mathcal{R}_3(w';\hat{v}, \hat{p}) \) is obtained by setting \( \hat{v} = \bar{v} + v' \) in the definition of the residual given in (2.19).

The solution of the weak form of nonlinear equations is accomplished via iterative schemes that are based on the solution of a sequence of linearized problems. Therefore, for clarity of presentation we introduce an iteration counter expressed as \( (\bullet)^{(i)} \). For the sake of simplicity, we consider that linearization is done about the last converged coarse-scale solution, i.e., \( \hat{v} \approx \bar{v}^{(i)} \). Keeping the \( \partial \bar{v}' \) terms on the left hand side and taking the \( \delta \bar{v} \) terms on to the right hand side we get:
\[ (w', \delta v' \cdot \nabla \tilde{v}^{(i)} + \tilde{v}^{(i)} \cdot \nabla \delta v') + \beta (w', \tilde{v}^{(i)} \nabla \cdot \delta v' + \delta v' \cdot \nabla \tilde{v}^{(i)}) + (\nabla \cdot w', 2\nu \nabla \delta v') \]
\[ = - \mathcal{R}_3(w'; \tilde{v}, p)^{(i)} - (w', \delta \tilde{v}) - (w', \delta \tilde{v} \cdot \nabla \tilde{v}^{(i)} + \tilde{v}^{(i)} \cdot \nabla \delta \tilde{v}) \]
\[ - \beta (w', \tilde{v}^{(i)} \cdot \delta \tilde{v} + \delta \tilde{v} \cdot \nabla \tilde{v}^{(i)}) + (w', 2\nu \Delta \delta \tilde{v}) + (\nabla \cdot w', \delta p) \]
\[ = -(w', r) \]

where \( \Delta (\bullet) \) is the Laplacian operator. The residual \( r \) on the right hand side of (2.22) can be decomposed into \( r_1 \) and \( r_2 \) as:

\[ r = r_1(\tilde{v}^{(i)}, p^{(i)}) + r_2(\delta \tilde{v}, \delta p, \tilde{v}^{(i)}) \] (2.23)

where

\[ r_1(\tilde{v}^{(i)}, p^{(i)}) = (\tilde{v}_\nu + \tilde{v} \cdot \nabla \tilde{v} + \beta \tilde{v} \nabla \cdot \tilde{v} - 2\nu \Delta \tilde{v} + \nabla p - f)^{(i)} \] (2.24)

and

\[ r_2(\delta \tilde{v}, \delta p, \tilde{v}^{(i)}) = (\tilde{v}_\nu + \tilde{v} \cdot \nabla \tilde{v} + \beta \tilde{v} \nabla \cdot \tilde{v} - 2\nu \Delta \tilde{v} + \nabla p - f)^{(i)} \] (2.25)

The function \( r_1(\tilde{v}^{(i)}, p^{(i)}) \) defined in (2.24) is the residual of the Euler-Lagrange equations, and \( r_2(\delta \tilde{v}, \delta p, \tilde{v}^{(i)}) \) defined in (2.25) is the incremental residual emanating from the linearization of the nonlinear fine-scale problem. Therefore the fine-scale problem described via equation (2.22) is a residual driven problem, where fine scales evolve to account for the lack of resolution in the coarse scales. During nonlinear iterations in a generic time step, \( r_2(\delta \tilde{v}, \delta p, \tilde{v}^{(i)}) \) converges to zero within a predefined tolerance, and consequently, the converged fine scales become a function of the residual of the Euler-Lagrange equations for the coarse scales alone.

Our objective at this point is to solve (2.22) to extract the fine-scale solution \( \delta v' \) that can then be substituted in the coarse-scale sub-problem. If we assume that the fine scales \( \delta v' \) and \( w' \) are represented via bubble functions \( b^c(\xi) \) over \( \Omega' \), then substituting them in (2.22) and following the procedure in Masud and Khurram [92] and Masud and Franca [95], we recover a local problem defined over the sum of element interiors. The solution of the local problem yields the reconstructed fine-scale field:
\[
\delta v'(x) = -b^e + \beta \int b^e \bar{v}^{(i)} \otimes \nabla b^e \, d\Omega + \beta \int b^e (\nabla \cdot \bar{v}^{(i)}) \, d\Omega I
\]

where \( I \) is the \( n_{sd} \times n_{sd} \) identity matrix and \( n_{sd} \) represents the number of spatial dimensions. Without any loss of generality we assume a piecewise constant projection of the residual \( r \) over the element interiors, thereby yielding the following simplified form for the fine scales:

\[
\delta v'(x) = -\tau r
\]

The stabilization operator \( \tau \) is defined as

\[
\tau = b^e \int b^e d\Omega + \beta \int b^e \bar{v}^{(i)} \otimes \nabla b^e d\Omega + \beta \int b^e (\nabla \cdot \bar{v}^{(i)}) d\Omega I
\]

Remark: In this approach fine scales are being solved in a direct nonlinear fashion.

Remark: During nonlinear iterations in any given time step the residual \( r_2(\delta \bar{v}, \delta p, \bar{v}^{(i)}) \) converges to zero. Consequently the fine scale increments \( \delta v'(x) \) become function of the residual \( r_1(\bar{v}^{(i)}, p^{(i)}) \), which is the residual of the Euler-Lagrange equations for the coarse scales alone.

Remark: Assuming a piecewise constant projection of the residual \( r \) in (2.27) amounts to employing a mean value of the residual over the element interiors.

2.3.3 Solution of the coarse-scale sub-problem

Let us now consider the weak form of the coarse-scale sub-problem for the momentum equation (2.17). We take variational derivative of the nonlinear operator \( R_1(\cdot, \cdot) \) to obtain the linearized operators \( L(R_1(\cdot, \cdot)) \):

\[
\int (b^e)^2 \nabla^T \bar{v}^{(i)} \, d\Omega + \int b^e \bar{v}^{(i)} \cdot \nabla b^e \, d\Omega I
\]
\[ L \left( \mathcal{R}_i(\vec{w}; \vec{v}', p) \right) \overset{\text{def}}{=} \frac{d}{d\varepsilon} \mathcal{R}_i(\vec{w}; \vec{v} + \varepsilon \delta \vec{v}, \vec{v}' + \varepsilon \delta \vec{v}', p + \varepsilon \delta p) \bigg|_{\varepsilon=0} \]  

Applying (2.29) to (2.17), linearizing about the known solution \( \hat{v} \) and \( \hat{p} \), and dropping the higher order terms we get,

\[
(\vec{w}, \delta \vec{v}) + (\vec{w}, (\delta \vec{v} + \delta \vec{v}') \cdot \nabla \hat{v} + \hat{v} \cdot \nabla (\delta \vec{v} + \delta \vec{v}')) \\
+ \beta (\vec{w}, (\delta \vec{v} + \delta \vec{v}') \nabla \cdot \hat{v} + \hat{v} \cdot (\delta \vec{v} + \delta \vec{v}')) \\
+ (\nabla' \vec{w}, 2v \nabla^s (\delta \vec{v} + \delta \vec{v}')) - (\nabla \cdot \vec{w}, \delta \varepsilon) = - \mathcal{R}_i(\vec{w}; \hat{v}, \hat{p})
\]  

where \( \mathcal{R}_i(\vec{w}; \hat{v}, \hat{p}) \) is obtained from the definition of the residual in (2.17) by setting \( \hat{v} = \vec{v} + \vec{v}' \).

For the sake of simplicity we follow along the lines of the fine scale problem and consider that linearization is done about the last converged coarse-scale solution, i.e., we set \( \hat{v} \approx \vec{v}^{(i)} \). Exploiting linearity of the solution slot we get:

\[
(\vec{w}, \delta \vec{v}) + (\vec{w}, \delta \vec{v} \cdot \nabla \vec{v}^{(i)}) + (\vec{w}, \delta \vec{v}' \cdot \nabla \vec{v}^{(i)}) + (\vec{w}, \vec{v}^{(i)} \cdot \nabla \delta \vec{v}) \\
+ (\vec{w}, \vec{v}^{(i)} \cdot \delta \vec{v}') + \beta (\vec{w}, \delta \vec{v}' \cdot \nabla \vec{v}^{(i)}) + \beta (\vec{w}, \delta \vec{v}' \cdot \nabla \vec{v}^{(i)}) \\
+ \beta (\vec{w}, \vec{v}^{(i)} \cdot \delta \vec{v}) + \beta (\vec{w}, \vec{v}^{(i)} \cdot \nabla \delta \vec{v}') + (\nabla' \vec{w}, 2v \nabla^s \delta \vec{v}') \\
+ (\nabla' \vec{w}, 2v \nabla^s \delta \vec{v}')(\delta \vec{v}') - (\nabla \cdot \vec{w}, \delta \varepsilon) = - \mathcal{R}_i(\vec{w}; \vec{v}, p)^{(i)}
\]  

Integrating by parts the terms (a), (b) and (c) in (2.31) and exploiting the assumption that fine scales \( \partial \vec{v}' \) vanish on the boundaries of the elements we get, respectively:

\[
(\vec{w}, \vec{v}^{(i)} \cdot \nabla \delta \vec{v}') = - (\nabla \cdot \vec{v}^{(i)} \vec{w}, \delta \vec{v}') - (\vec{v}^{(i)} \cdot \nabla \vec{w}, \delta \vec{v}')
\]  

\[
\beta (\vec{w}, \vec{v}^{(i)} \cdot \delta \vec{v}') = - \beta (\vec{w}, \delta \vec{v}' \cdot \nabla \vec{v}^{(i)}) - \beta (\delta \vec{v}' \cdot \nabla \vec{w}, \vec{v}^{(i)})
\]  

\[
(\nabla' \vec{w}, 2v \nabla^s \delta \vec{v}')(\delta \vec{v}') = - (\Delta \vec{w}, 2v \delta \vec{v}')
\]  

where the operator \( \Delta \) in equation (2.34) is the vector Laplacian operator. Substituting (2.32)-(2.34) and the fine scale solution \( \delta \vec{v}' \) given by (2.27) in (2.31) we get:
\[(\bar{w}, \delta\bar{v}) + (\bar{w}, \delta\bar{v} \cdot \nabla \bar{v}^{(i)} + \bar{v}^{(i)} \cdot \nabla \delta\bar{v}) + \beta (\bar{w}, \bar{v}^{(i)} \nabla \delta v + \delta v \nabla \bar{v}^{(i)}) + (\nabla' \bar{w}, 2v\nabla' \delta\bar{v}) - (\bar{v}, (1 - \beta)(\tau r) \cdot \nabla \bar{v}^{(i)}) + \beta ((\tau r) \cdot \nabla \bar{w}, \bar{v}^{(i)}) = - \mathcal{R}_2(\bar{w}; \bar{v}, p)^{(i)} \]  

(2.35)

We now consider the residual \(\mathcal{R}_2(q; \bar{v}, v')\) of the continuity equation and take the variational derivative:

\[\mathcal{L}(\mathcal{R}_2(q; \bar{v}, v')) \overset{def}{=} \frac{d}{d\varepsilon} \mathcal{R}_2(q; \bar{v} + \varepsilon \delta \bar{v}, v' + \varepsilon \delta v') \bigg|_{\varepsilon = 0} \]  

(2.36)

Applying (2.36) to the continuity equation (2.18) we get:

\[(q, \nabla \cdot (\delta\bar{v} + \delta v')) = - \mathcal{R}_2(q; \hat{v}) \]  

(2.37)

where \(\mathcal{R}_2(q; \hat{v})\) is obtained from the definition of the residual given in (2.18). As was done for the momentum equation above, we set \(\hat{v} \approx \bar{v}^{(i)}\), and substitute \(\delta v'\) from (2.27) in (2.37) to obtain the residual form of the weak form of the continuity equation:

\[(q, \nabla \cdot \delta\bar{v}) + (\nabla q, \tau r) = - \mathcal{R}_2(q, \bar{v})^{(i)} \]  

(2.38)

We can now combine (2.35) and (2.38) to develop the variational multiscale residual-based stabilized form for the incompressible Navier-Stokes equations. Since the resulting equation is expressed entirely in terms of the coarse scales, for the sake of simplicity the superposed bars are dropped:

\[\begin{align*}
(w, \delta v) + (w, \delta v \cdot v^{(i)}) + v^{(i)} \cdot \nabla v) + \beta (w, v^{(i)} \nabla \delta v + \delta v \nabla v^{(i)})
+ (\nabla' w, 2v\nabla' \delta v)
- (\nabla \cdot w, \delta p) + (q, \nabla \cdot v)
+ (v^{(i)} \cdot \nabla w + 2v\Delta w + \nabla q + (1 - \beta)w \nabla v^{(i)}, \tau r_2)
- (1 - \beta)(w, (\tau r_2) \cdot \nabla v^{(i)}) + \beta ((\tau r_2) \cdot \nabla w, v^{(i)})
\end{align*} \]

(2.39)

Stabilization terms

\[= - \mathcal{R}_1(w; v, p)^{(i)} - \mathcal{R}_2(q; v)^{(i)}
- (v^{(i)} \cdot \nabla w + 2v\Delta w + \nabla q + (1 - \beta)w \nabla v^{(i)}, \tau r_1)
+ (1 - \beta)(w, (\tau r_1) \cdot \nabla v^{(i)}) - \beta ((\tau r_1) \cdot \nabla w, v^{(i)})
\]

Stabilization terms

where \(r_1(v^{(i)}, p^{(i)})\) and \(r_2(\delta v, \delta p, v^{(i)})\) are the residuals defined in equations (2.24) and (2.25), respectively.
Remark: Considering $\hat{v} = \vec{v}^{(i)} + v^{*(i)}$ instead of $\hat{v} \approx \vec{v}^{(i)}$ would introduce the fine-scale and cross-advection terms that are present in the turbulence formulations that are derived in the context of the Variational Multiscale method [10].

Remark: The left hand side of (2.39) yields the consistent tangent for the new stabilized formulation, where contributions from both the coarse and fine scales are present. However it is important to note that the consistent tangent is explicitly written in terms of the coarse scale variables.

2.3.4 The nonlinear stabilized form

The nonlinear stabilized form is given by the nonlinear residual on the right hand side of (2.39) together with the consideration that solution to (2.39) is attained when the left hand uniformly converges to zero. In addition, when convergence is attained, superposed indices $(\cdot)^{(i)}$ can be dropped and the nonlinear variational form for the new stabilized method can be written as:

$$
\begin{align*}
& \mathcal{R}_1(w; v, p) + \mathcal{R}_2(q; v) \\
& + \left( v \cdot \nabla w + 2\nu \Delta w + \nabla q + (1-\beta)w \nabla \cdot v \tau_r \right) \\
& - (1-\beta)(w, (\tau_r) \cdot \nabla v) + \beta((\tau_r) \cdot \nabla w, v) = 0
\end{align*}
$$

This nonlinear formulation can be rewritten in terms of the Galerkin terms and the additional stabilization terms. The appropriate space of function for the pressure field for this new formulation is $p \in \mathcal{P} = H^1(\Omega)$.

2.3.4.1 The stabilized momentum conservation form

Setting $\beta = 1$ leads to the stabilized momentum conservation form as follows:

$$
\begin{align*}
& (w, v_r) + (w, \nabla \cdot (v \otimes v)) + (\nabla' w, 2\nu \nabla' v) - (\nabla \cdot w, p) + (q, \nabla \cdot v) \\
& + \left( v \cdot \nabla w + 2\nu \Delta w + \nabla q \cdot \tau_r \right) + ((\tau_r) \cdot \nabla w, v) = (w, f) + (w, h)_{\tau_r}
\end{align*}
$$

2.3.4.2 The stabilized non-conservative form

Setting $\beta = 0$ leads to the stabilized non-conservative form as follows:
\[(w, v) + (w, v \cdot \nabla v) + (\nabla^T w, 2v \nabla^T v) - (\nabla \cdot w, p) + (q, \nabla \cdot v) + (v \cdot \nabla w + 2v \Delta w + \nabla q, \tau \nabla v) + (w \nabla \cdot v, \tau \nabla v) + (w, (\tau \cdot \nabla) \cdot \nabla v) \]
\[= (w, f) + (w, h)_{1, h} \tag{2.42} \]

Remark: In our numerical implementation presented in the Sec. 2.5, we have adopted the stabilized non-conservative form.

Remark: The variational multiscale based stabilized form possesses additional stabilization terms than are provided by the classical stabilization methods alone.

2.4 Structure of the stabilization tensor

The structure of the stabilization tensor \( \tau \) is derived via the solution of the fine-scale sub-problem (2.19). It is important to note that if we use same bubble functions for the fine-scale solution and fine-scale weighting function in the skew advection terms in (2.28), these terms cancel out. In order to retain the contribution from the skew terms, we employ the idea proposed in [89, 92] and we use bubble functions of a different order in the weighting function slot in these terms. We indicate by \( b_2^f(\xi) \) the bubble functions that are employed for the weighting function in the skew terms and by \( b_1^e(\xi) \) the bubble functions that are used in the expansion of all other fine-scale trial solutions and weighting functions. Accordingly, we write (2.28) in terms of these two different bubble functions:

\[
\tau = b_1^e \int_{\Omega} b_1^e d\Omega \left[ \int \left( b_1^e \right)^2 \nabla^T v \cdot d\Omega + \int b_1^e \nabla \cdot \nabla b_1^e \d\Omega + \beta \int b_1^e \nabla \cdot \nabla b_1^e \d\Omega \right]^{-1}
\]

\[
+ \beta \int b_1^e \nabla \cdot v \d\Omega + v \int \left| \nabla b_1^e \right|^2 \d\Omega + v \int \nabla b_1^e \otimes \nabla b_1^e \d\Omega \tag{2.43} \]

In our numerical implementation presented in Sec. 2.5, \( b_1^e(\xi) \) is the standard quadratic bubble for the linear brick and tetrahedral elements as well as for the quadratic tetrahedral element. However, this standard quadratic bubble is not appropriate for the quadratic brick element (27-noded brick) because it linearly depends on the shape function for the central node of the element. Therefore, for quadratic bricks we use a 4th order bubble function.
The bubble \( b^e_2(\xi) \) that is used in the fine scale weighting function in the skew term is taken to be the shape function corresponding to the vertex that provides the most up-winding in the element. This idea has been motivated by the residual-free bubble (RFB) method proposed by Brezzi et al. [18], wherein an element wise problem is solved to design the residual free bubble. The simplifying the steps in [18] yields values of \( \tau \) that are a function of a scalar parameter that represents the location of the internal node. In the present work we define the bubble \( b^e_2(\xi) \) in terms of the vertex node that provides most up-winding in the element. A 2D schematic representation of the idea is shown in Fig. 2.1. Since the vertex node that provides up-winding effects can potentially change in transient calculations due to a local change in the direction of the flow field, we propose a simple and economic procedure to identify the vertex node that is used to describe \( b^e_2(\xi) \) in the calculations. Our approach is based on the following algorithm. We first compute the center point of the element and associate with this point a vector \( v_b \) that is obtained by averaging over the element the nodal velocity \( \bar{v}^{(i)} \) from the previous iteration. Then we determine the angles between \( v_b \) and the direction vectors that join the center point of the element to each of its vertices. The most upstream vertex is identified to be the one that maximizes the angle. If there are more than one vertex nodes with the same maximum angle, then the vertex node that maximizes the distance from the center point of the elements is chosen to define the bubble function \( b^e_2(\xi) \).

**Remark 9:** The definition of stabilization tensor \( \tau \) presented in (2.43) leads to a full matrix, thus bringing in cross coupling effects in the stabilization terms. These cross coupling effects are not present in the standard GLS or SUPG methods (see e.g., [89]).

In the context of a given velocity field that leads to an advective-diffusive system, one can quantify the flow regime in terms of the Peclet number \( (Pe) \), i.e. low \( Pe \) represents diffusion dominated flow and high \( Pe \) indicates advection dominated flow. To analyze the behavior of the stabilization tensor \( \tau \) in the two flow regimes, we write it as:

\[
\tau = b^e_1 \int b^e_1 \text{d} \Omega \left( \hat{\tau}^{adv} + \hat{\tau}^{diff} \right)^{-1}
\]

(2.44)
where \( \hat{\tau}^{adv} \) and \( \hat{\tau}^{diff} \) are the advection and diffusion contributions to the stabilization tensor, respectively. Equation (2.44) can be further made concise as \( \tau = \hat{b}^e \hat{\tau} \). Tables 1 and 2 show the magnitude of these tensors for low and high convective velocity fields, respectively. We define the magnitude of a second order tensor \( \tau \) as \( \sqrt{\tau : \tau} \). In all the test cases, the convective velocity forms an angle of 30° with the \( z \)-direction and an angle of 23.4° with the \( y-z \) plane. The magnitude of the stabilization tensors for various element types as a function of mesh refinement are shown in Tables 1 and 2. These tables show that the magnitude of the advection component of the stabilization tensor decreases with increasing the order of the interpolation functions used, which is consistent with the studies conducted in Akin and Tezduyar [1] that are based on the stabilization parameters introduced in Tezduyar and Park [123].

In addition, we see that the norm of \( \hat{\tau} \), which contains both \( \hat{\tau}^{adv} \) and \( \hat{\tau}^{diff} \), is smaller in magnitude for high \( Pe \) flows as compared to its value for low \( Pe \) flows for each of the element types considered in Tables 1 and 2.

**Remark:** In our numerical simulations presented in Sec. 2.5, we have employed the full stabilization tensor \( \tau \) that emanates from the solution of the fine-scale problem and is presented in equation (2.43). The segregated form shown in equation (2.44) was for the purpose of analyzing the contributions from the advective and diffusive components of the full stabilization tensor for various flow regimes.

### 2.5 Numerical results

In our numerical implementation we have adopted the stabilized non-conservative form presented in equation (2.42) and therefore \( \beta = 0 \) in all the numerical tests presented in this section. Acceptable tolerance to reach convergence in nonlinear iterations is set to be \( 10^{-10} \). A family of linear and higher order tetrahedral and hexahedral elements with equal-order pressure-velocity interpolations (see Fig. 2.2) has been developed, and full numerical quadrature is employed in all the element types.

This section is divided in two parts. The first part presents a study of the numerical convergence rates for the proposed stabilized formulation. The second part employs the lid-
driven cavity problem which is a standard benchmark test case to investigate the stability and engineering accuracy of the computed solutions.

2.5.1 Rate of convergence study

The first set of numerical simulations presents the convergence rates for the stabilized formulation presented in equation (2.42). The domain under consideration is a cube of unit length, centered at $x = 0.5$, $y = 0.5$ and $z = 0.5$. Kinematic viscosity $\nu = 1$. The exact solution of the problem is a Beltrami flow given by Ethier and Steinman [32]:

\begin{align*}
\nu_x &= - e^x \sin(y + 2z) - e^z \cos(x + 2y) \\
\nu_y &= - e^y \sin(z + 2x) - e^x \cos(y + 2z) \\
\nu_z &= - e^z \sin(x + 2y) - e^y \cos(z + 2x) \\
p &= - \frac{1}{2} (e^{2x} + e^{2y} + e^{2z}) - \sin(x + 2y) \cos(z + 2x) e^{x+z} \\
&\quad - \sin(y + 2z) \cos(x + 2y) e^{y+z} - \sin(z + 2x) \cos(y + 2z) e^{x+y}
\end{align*}

(2.45)

Figure 2.3 shows the contour plots of the exact solution. The body force that drives the problem is derived by substituting (2.45) in (2.1). For the numerical problem, we prescribe the exact velocity boundary conditions at the boundaries. In addition, we prescribe the exact pressure at one of the vertices of the domain.

The meshes employed for the rate of convergence study consist of $10^3$, $15^3$, $20^3$ and $30^3$ elements for the case of linear bricks, and $5^3$, $15^3$ and $20^3$ elements for the case of quadratic bricks. The corresponding tetrahedral meshes are obtained by dividing each brick element into 6 tetrahedrons.

The convergence rate study is divided into two parts:

(i) The first part of this study investigates the convergence properties of the Stokes part of the formulation that is obtained by setting the skew advection terms equal to zero in the stabilized formulation given in (2.42).

(ii) The second part of this study investigates the convergence rates for the linearized Navier-Stokes equations for both low and high convective velocities.
In addition, in both convergence studies we also investigate the attributes of accurately evaluating the second order terms that appear in the stabilization operators of the formulation given in equation (2.42).

2.5.1.1 Convergence study for the Stokes part of the formulation

If the transient and convective terms are dropped form (2.42), the formulation reduces to the stabilized form for the steady Stokes equations:

\[ (\nabla' w, 2v\nabla' v) - (\nabla \cdot w, p) + (q, \nabla \cdot v) + (2v\Delta w + \nabla q, \tau(-2v\Delta v + \nabla p - f)) = (w, f) + (w, h)_{\Gamma_h} \tag{2.46} \]

Moreover, for the Stokes problem the stabilization tensor \( \tau \) (2.43) that emanates from the solution of the corresponding fine-scale problem reduces to:

\[ \tau = b^e \int b^e d\Omega \left[ \nu \int \| \nabla b^e \|^2 d\Omega I + \nu \int \nabla b^e \otimes \nabla b^e d\Omega \right]^{-1} \tag{2.47} \]

Figure 2.4(a-d) presents the convergence rates in terms of the \( L_2 \)-norm of the velocity field and \( H_1 \)-norm of the pressure field for all the element types considered. The convergence rates for the Stokes operator, employing linear elements is given in [59], where it is shown that optimal rates are

\[ \| e_v \| = O(\tau^2) \tag{2.48} \]

and

\[ \| \nabla e_v \| = O(\tau^{0.5}) \tag{2.49} \]

Since second order derivatives vanish for the linear elements, the discrete problem is consistent and therefore optimal convergence rates are attained for the velocity field. However, if second derivatives are not evaluated for the higher order elements, the discrete problem lacks consistency and therefore computed convergence rates for the velocity field are sub-optimal. In the context of 2D formulations, similar effects of the second derivatives on the convergence rates for quadratic triangles and quadrilaterals were observed in Masud and Khurram [92].
2.5.1.2 Convergence study for the linearized Navier-Stokes equations

This section presents the convergence rate study for the stabilized form of the linearized Navier-Stokes equations. The convective velocity $v^c$ is assumed given, and is considered constant over the computational domain. Furthermore, the convective velocity $v^c$ is not taken to be parallel to any of the characteristic directions of the mesh so that the computed rates reflect the convergence properties for a general flow regime. In particular we consider two cases, $|v^c| = 40$ ($v_x = 17.31$, $v_y = 10$, and $v_z = 34.64$) and $|v^c| = 400$ ($v_x = 173.1$, $v_y = 100$, and $v_z = 346.4$). Note that the exact solution for the present problem is the same as given in (2.45). However, in order to accommodate the new convective terms, we modify the body force term because $v^c$ is now considered a part of the given data.

Figures 2.5(a-d) and 2.6(a-d) present the $L_2$-norm of the velocity and $H_1$-norm of the pressure field for $|v^c| = 40$ and $|v^c| = 400$, respectively. As stated earlier, if the second derivatives are not evaluated in the calculation of the stabilization terms for the higher order elements, sub-optimal convergence rates are observed.

2.5.2 Lid-driven cavity flow

Lid-driven cavity problem is widely used as a benchmark problem for studying the stability and engineering accuracy of formulations for the incompressible Navier-Stokes equations. In this section we present two sets of numerical results. First we present results for a bi-dimensional driven cavity flow and we compare our results with the 2D results obtained by Ghia and co-workers [45] where authors have used a multigrid method in the context of finite difference calculations. Then we present results for the full 3D lid-driven cavity problem, and these results are compared with those obtained by Jiang and co-workers [71] where authors have employed a least-squares based finite element method.

2.5.2.1 Two-dimensional lid-driven cavity flow

The two-dimensional flow is modeled on a hexahedral domain with bi-unit square cross section and a thickness equal to $9 \times 10^{-3}$ (see Fig. 2.7). A unit tangential velocity in the $x$-direction is applied at the top surface of the computational domain. In addition, zero
pressure is prescribed at one of the corner points. The domain is discretized with a graded mesh of 43,350 tetrahedral elements that are spread as a 2D mesh with just one element through the thickness direction. Due to the nonlinear character of the problem, the tangential velocity \( v_x \) is gradually increased from 0 to 1 in 100 equal load steps. The acceptable tolerance to achieve convergence is set equal to \( 10^{-10} \).

Numerical simulations are carried out for three values of viscosity, \( \nu = 0.001 \) (\( \text{Re} = 1,000 \)), \( \nu = 0.0002 \) (\( \text{Re} = 5,000 \)) and \( \nu = 0.0001 \) (\( \text{Re} = 10,000 \)). In this problem, a main vortex appears in the center of the cavity (see Fig. 2.8), and depending on the Reynolds number, additional vortices appear in the corners of the cavity. Results in Fig. 2.8 compare well with the results presented in Ghia \textit{et al.} [45] for the corresponding Reynolds number flows.

Figure 2.9 presents line plots of the horizontal velocity at a vertical line \((x = 0.5, z = 0)\) and these are compared with the results presented in [45]. Once again results match very well and good engineering accuracy is attained in all the three cases.

In Sec. 2.3, we presented the consistent tangent for the Navier-Stokes equations that was derived within the variational multiscale framework. Table 3 shows quadratic convergence of the Newton-Raphson scheme with the consistent tangent for \( \text{Re} = 5,000 \).

2.5.2.2 \textit{Three-dimensional lid-driven cavity flow}

The second set of results for the lid-driven cavity problem simulate the full three dimensional effects. We consider a cube of unit volume (see Fig. 2.10) centered at \( x = y = z = 0.5 \). A unit tangential velocity in the \( x \)-direction is prescribed at the top surface \((y = 1)\) while zero velocity is prescribed on the remaining bounding surfaces. Pressure boundary condition is prescribed at \((x, y, z) = (0, 0, 0.5)\) where pressure is set equal to zero. Since the computational domain and the boundary conditions are symmetric with respect to the \( x \)-\( y \) plane passing through \( z = 0.5 \), only one half of the domain is discretized with a graded mesh of 8-noded brick elements (30 in the \( x \)- and \( y \)-directions and 15 in the \( z \)-direction). This test problem is repeated with a mesh of tetrahedral elements to show the applicability of the formulation to general element types. This tetrahedral mesh is constructed by dividing each of the brick elements into six tetrahedrons.
In this general 3D flow problem, we have considered three values of the viscosity, \( \nu = 0.01 \), \( \nu = 0.001 \) and \( \nu = 0.0005 \), which correspond to \( Re = 100 \), \( Re = 1000 \) and \( Re = 2000 \), respectively.

Like the bi-dimensional case, the resulting flow contains a main vortex in the center of the domain (Figs. 2.11(a), 2.12 and 2.13). This main vortex is parallel to the \( x-y \) plane. However, the no-slip condition on the lateral walls (\( z = 0 \) and \( z = 1 \)) produces out-of-plane vortices in the third dimension (Figs. 2.11(c), 2.11(e), 2.12 and 2.13). Stream-vectors and pressure contours in Fig. 2.11 compare well with the results presented in Jiang and co-workers [71] where authors have used non-uniform meshes of 50\( \times \)52\( \times \)25 tri-linear elements.

Figures 2.12(a) and 2.12(b) show the streamlines for \( Re = 1,000 \) and \( Re = 2,000 \), respectively. For \( Re = 2,000 \) the effects of out-of-plane vortices are more significant and these are the source of turbulence in flows at higher Reynolds numbers. Figures 2.13(a) and 2.13(b) show velocity vectors and pressure iso-surfaces for \( Re = 1,000 \), and \( Re = 2,000 \), respectively.

Figures 2.14(a-b) show the line plots of the \( x \)-velocity for the brick mesh at a vertical line passing through the center of the cavity for the \( Re = 100 \) and \( Re = 1,000 \) cases, respectively. Once again our results are in a good agreement with the results reported in [71].

**Remark:** It is important to note that our results are reported on meshes that contain about one fifth degrees of freedom as compared to Jiang et al. [71]. This results in two orders of magnitude reduction in the computational cost for an equivalent engineering accuracy.

The results obtained for the tetrahedral mesh are very similar to the ones obtained for the brick element mesh. Figure 2.15 shows a comparison of the results obtained for the two mesh types for \( Re = 1,000 \). Since the simulations for the tetrahedral mesh do not furnish any additional information, further results are not shown.

### 2.6 Conclusions

We have presented a Variational Multiscale based stabilized formulation for the incompressible Navier-Stokes equations. A novel feature of our method is that fine scales are solved in a direct nonlinear fashion. Consistent linearization of the nonlinear equations in the
context of the Variational Multiscale framework leads to the design of the stabilization terms in the new method. The VMS based stabilized form possesses additional stabilization terms than are present in the classical stabilization methods alone. An important feature of the new method is that a definition of the stabilization operator $\tau$ appears naturally via the solution of the fine-scale problem. This stabilization operator is a second order tensor and leads to a full matrix that brings in cross coupling effects in the stabilization terms. A computationally economic scheme is proposed that incorporates up-winding effects in the calculation of the advection part of the stabilization operator $\tau$. Good stability and accuracy properties of the new method are shown for a family of linear and quadratic tetrahedral and hexahedral elements.

2.7 Figures and tables

![Schematic representation of the procedure for choosing the most up-winding vertex](image)

**Figure 2.1** Schematic representation of the procedure for choosing the most up-winding vertex
Figure 2.2 Family of 3D linear and higher order elements

(a) 8 node brick  (b) 4 node tetrahedron

(c) 27 node brick  (d) 10 node tetrahedron

Figure 2.3 Exact solution to the problem employed for the convergence study, (a) Velocity field, and (b) Pressure field
Figure 2.4 Convergence rates for the Stokes equations
Figure 2.5 Convergence rates for the linearized Navier-Stokes equations ($|\psi^v| = 40$)
Figure 2.6 Convergence rates for the linearized Navier-Stokes equations $(|v^*| = 400)$
Figure 2.7 (a) Schematic diagram of the equivalent 2D lid-driven cavity flow problem. (b) Sample of a graded mesh composed of 4-noded tetrahedral elements
Figure 2.8 Streamlines for the bi-dimensional flow using 4-noded tetrahedral elements for
(a) $Re = 1,000$, (b) $Re = 5,000$ and (c) $Re = 10,000$
Figure 2.9 Comparison of our results with Ghia et al. [45] at (a) Re = 1,000, (b) Re = 5,000 and (c) Re = 10,000

Figure 2.10 Schematic diagram of the 3D lid-driven cavity problem
(a) Flow pattern at $z = 0.5$

(b) Pressure contours at $z = 0.5$

(c) Flow pattern at $x = 0.5$

(d) Pressure contours at $x = 0.5$

(e) Flow pattern at $y = 0.5$

(f) Pressure contours at $y = 0.5$

**Figure 2.11** Sections of the flow pattern and pressure contour for the 3D lid-driven cavity problem using 8-node brick elements ($Re = 1,000$)
Figure 2.12 Streamlines for 8-node brick elements at (a) Re = 1,000, and (b) Re = 2,000 (only the symmetric part is presented). This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.
Figure 2.13 Pressure iso-surfaces and stream-vectors for the 3D lid-driven cavity problem using 8-node brick elements. (a) Re = 1,000, and (b) Re = 2,000. This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.
Figure 2.14 Comparison with results from Jiang et al. [71] at (a) \( \text{Re} = 100 \), and (b) \( \text{Re} = 1,000 \)

Figure 2.15 Comparison of results for the two considered meshes. \( \text{Re} = 1,000 \)
Table 2.1 Magnitude of the stabilization tensor for various element types for low Peclet number flows.

\[ Pe = \left| \nu \right| \frac{h}{2\nu}, \nu = 1, \beta = 0 \text{ and } \left| \nu \right| = 40 \]

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<th>4-noded tetrahedron</th>
<th>10-noded tetrahedron</th>
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</table>
Table 2.2 Magnitude of the stabilization tensor for various element types for high Peclet number flows. $Pe = \frac{v^c h}{2\nu}$, $\nu = 1$, $\beta = 0$ and $v^c = 400$

| $|v^c| = 400$ | 8-noded brick | 27-noded brick | 4-noded tetrahedron | 10-noded tetrahedron |
|----------------|----------------|----------------|---------------------|---------------------|
| $h = 1/10$ $Pe = 20.0$ | $\|\hat{\tau}_{adv}\|$ | $7.95 \times 10^1$ | $7.79 \times 10^2$ | $5.45 \times 10^1$ | $2.92 \times 10^2$ |
|                       | $\|\hat{\tau}_{diff}\|$ | $1.01$ | $3.20$ | $7.44 \times 10^1$ | $7.44 \times 10^1$ |
|                       | $\|\vec{r}\|$ | $4.82 \times 10^4$ | $4.68 \times 10^4$ | $1.21 \times 10^4$ | $2.08 \times 10^4$ |
| $h = 1/15$ $Pe = 13.3$ | $\|\hat{\tau}_{adv}\|$ | $3.53 \times 10^1$ | $3.45 \times 10^2$ | $2.42 \times 10^1$ | $1.30 \times 10^2$ |
|                       | $\|\hat{\tau}_{diff}\|$ | $7.01 \times 10^1$ | $2.14$ | $4.96 \times 10^1$ | $4.96 \times 10^1$ |
|                       | $\|\vec{r}\|$ | $2.50 \times 10^4$ | $2.10 \times 10^4$ | $6.30 \times 10^5$ | $9.36 \times 10^5$ |
| $h = 1/20$ $Pe = 10.0$ | $\|\hat{\tau}_{adv}\|$ | $1.99 \times 10^1$ | $1.95 \times 10^2$ | $1.36 \times 10^1$ | $7.30 \times 10^3$ |
|                       | $\|\hat{\tau}_{diff}\|$ | $5.26 \times 10^1$ | $1.60$ | $3.72 \times 10^1$ | $3.72 \times 10^1$ |
|                       | $\|\vec{r}\|$ | $1.53 \times 10^4$ | $1.18 \times 10^4$ | $3.89 \times 10^5$ | $5.30 \times 10^5$ |

Table 2.3 Evolution of the relative magnitude of the residual for various load steps. $Re = 5,000$

<table>
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<th>Load step</th>
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<td>$1.00 \times 10^0$</td>
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<tr>
<td>4</td>
<td>$1.37 \times 10^{-12}$</td>
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Chapter 3

A multiscale stabilized ALE formulation for incompressible flows in problems with moving boundaries*

3.1 Motivation

Fluid mechanics problems that involve moving and deforming fluid-structure interfaces and/or free-surfaces can be observed in various engineering disciplines. The burgeoning interest in the modeling of biological flows, namely, the cardiovascular blood flow and the flow of air in the trachea and lungs has reignited great interest in the research community that is working in the area of flow-structure interaction problems. The two ingredients that are essential to the development of successful numerical techniques for this class of problems are: (i) a good numerical method that possesses superior stability and convergence properties, and as a pre-requisite, exhibits superior accuracy on fix grids, and (ii) a robust mesh moving technique that can update the spatially deforming computational grid without excessive local distortion of the elements as well as any degradation in the quality of the mesh. These two ingredients can then be coalesced via the arbitrary Lagrangian-Eulerian framework wherein the flow equations are integrated with the motion of the underlying continuum that appears as an additional independent field and needs to be solved for together with the flow variables.

In the last three decades, stabilized finite element methods have been developed and successfully applied to a variety of fluid flow problems. In the context of incompressible fluids, stabilized formulations are free of the Babuska-Brezzi $inf$-$sup$ condition on the combination of basis functions for the pressure and the velocity fields. In addition, stabilization also effectively controls the appearance of spurious oscillations in the advection

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dominated regions of the flow. The theoretical foundations of stabilized methods, namely the 
Streamline Upwind Petrov-Galerkin (SUPG) method [19, 58], and the Galerkin/Least-Squares (GLS) method [59, 63] were delineated by Hughes [64] via sub-grid scale modeling concept that laid the foundations of the Variational Multiscale (VMS) method [65]. Interested reader is directed to a review paper by Franca et al. [41] that describes the various stabilization approaches in the context of the advection-diffusion equation. Employing the VMS approach Masud and Hughes [87] developed new stabilized methods for the Darcy flow equations. These ideas were further extended by Masud and co-workers to derive the structure of stabilization terms as well as the structure of the stabilization tensor for a variety of physical problems; namely, convective-diffusive heat transfer [5], advection-diffusion equation [89], incompressible elasticity [90], and incompressible Navier-Stokes equations [92]. An important contribution in these works was the use of bubble functions in the expansion of the sub-grid scale problems that yield explicit structures of the stabilization tensors which can then be numerically computed via simple polynomials functions.

Moving boundary flow problems also require techniques to model the motion and deformation of the underlying fluid mesh. Various viewpoints have been pursued in the literature to develop good mesh moving techniques. Tezduyar and co-workers proposed solving modified elasticity equations wherein element Jacobian is excluded in the calculations, thereby introducing variable stiffening effect in the computational domain [127, 72, 73]. Masud and Hughes [86] proposed a method that is based on Galerkin/Least-Squares type modification of the Laplace equation that introduces spatially varying scalable-incompressibility effects in the computational domain. Though the motion of the fluid domain is considered “arbitrary” in the continuum ALE formulations, interestingly the situation is quite contrary in the discrete ALE formulations wherein the motion in the interior of the mesh is not completely arbitrary and is required to satisfy certain constraint conditions. In addition, the solution of the corresponding discrete system of equations can also suffer from the instabilities that are engendered by the mesh-motion based convective terms. Using advection-diffusion equation written in an ALE frame as a model problem, Masud [91] showed that if an arbitrary mesh motion results in an increase in the semi-norm of the relative velocity in the advection dominated regions of the flow, there is a corresponding drop in the accuracy of the solution because of a weaker bound on the growth of error. Analysis
presented in [91] also shows that mesh motion schemes need to satisfy certain constraint conditions in the interior of the mesh in addition to satisfying conditions at the deforming boundaries.

A literature review reveals that, in addition to the ALE based formulations for moving domain problems [57, 14], space-time finite element methods that accommodate the motion of the computational domain by slanting-in-time the space-time domain have also been successfully developed by Tezduyar et al. [124, 125] and Masud and Hughes [86]. In space-time methods the flow equations are written on slanted space-time slabs that account for the motion of the fluid domain as the problem evolves in time. A formal equivalence between the two approaches was established in [86]. Other approaches that have been applied to moving domain and flow-structure interaction problems encompass stabilized finite volume method [80], and particle finite element method [109]. Special time integration techniques for coupled field problems have been proposed in [34] that satisfy the so-called Geometric Conservation Laws [80] and thus preserve the superior properties of transient algorithms for deforming mesh problems.

The present work is an extension of our earlier works on stabilized methods for Navier-Stokes equations [92], extended to moving domain problems in [77]. In this work we integrate the multiscale/stabilized formulation developed in Masud and Calderer [97] with the mesh moving schemes [86, 94, 75] to solve problems involving moving and deforming fluid domains. An outline of the Chapter is as follows. Section 3.2 presents the Navier-Stokes equations written in an ALE frame. In Section 3.3 we derive the new stabilized method and the corresponding stabilization parameter. Section 3.4 provides a brief description of the mesh moving technique that is used in our simulations. In Section 3.5 we present an extensive set of numerical simulations for problems with fix as well as with moving boundaries. Conclusions are drawn in Section 3.6.
3.2 The incompressible Navier-Stokes equations in the ALE frame

Let \( \Omega_i \subset \mathbb{R}^{n_d} \) be a time-evolving open bounded region with piecewise smooth boundary \( \Gamma_i \). The number of space dimensions, \( n_d \), is equal to 3. The Arbitrary Lagrangian-Eulerian (ALE) form of the incompressible Navier-Stokes equations can be written as:

\[
\begin{align*}
\frac{\partial v}{\partial t} + (v - v^m) \cdot \nabla v - 2\nu \nabla \cdot \varepsilon(v) + \nabla p &= f & \text{in } \Omega_t \times ]0,T[ \\
\nabla \cdot v &= 0 & \text{in } \Omega_t \times ]0,T[ \\
v &= g & \text{on } \Gamma_g \times ]0,T[ \\
\sigma \cdot n &= (2\nu \varepsilon(v) - pI) \cdot n = h & \text{on } \Gamma_h \times ]0,T[ \\
v(x,0) &= v_0 & \text{on } \Omega_0 \times \{0\}
\end{align*}
\]

where \( v \) is the velocity vector, \( p \) is the kinematic pressure, \( f \) is the body force vector, \( \nu \) is the kinematic viscosity (assumed positive and constant), \( v^m \) is the fluid mesh velocity, \( I \) is the identity tensor, \( \varepsilon(v) \) represents the time derivative in the ALE frame, \( n \) is the exterior normal to the boundary \( \Gamma_i \), \( v_0 \) is the initial condition for the velocity field, and \( g \) and \( h \) are the Dirichlet and Neumann boundary conditions, respectively. \( \varepsilon(v) \) is the strain rate tensor, which is defined as \( \varepsilon(v) = \nabla v = (\nabla v + (\nabla v)^T)/2 \). Equation (3.1) represents the balance of momentum, equation (3.2) represents the continuity equation, equations (3.3) and (3.4) are the Dirichlet and Neumann boundary conditions, respectively, and equation (3.5) is the initial condition for the velocity field.

3.2.1 The standard weak form

Let \( w(x) \) and \( q(x) \) represent the weighting functions for the velocity and pressure fields, respectively. The appropriate spaces of weighting functions for these two fields are \( w \in V = (H^1_0(\Omega_i))^n_d \) and \( q \in P = C^0(\Omega_i) \cap L^2(\Omega_i) \), respectively. The appropriate spaces for
the velocity and pressure trial solutions are the corresponding time-dependent spaces $V_t$ and $P_t$. The standard weak form of the problem is

$$
\left( w, \frac{\partial v}{\partial t} \right)_y + \left( w, (v - v') \cdot \nabla v \right) + \left( \nabla' w, 2v \nabla' v \right) - \left( \nabla \cdot w, p \right) = (w, f) + (w, h)_{\Gamma_t} \tag{3.6}
$$

$$
(q, \nabla \cdot v) = 0 \tag{3.7}
$$

where $(\cdot, \cdot) = \int_\Omega (\cdot) d\Omega$ is the $L^2(\Omega_t)$-inner product.

**Remark:** Equations (3.6) and (3.7) represent the standard weak form of the problem, which in advection dominated flows lead to spurious oscillations in the pressure field. This issue is usually addressed via SUPG [19, 58] and GLS [59, 63] type methods.

In the following section we will develop a modified formulation that is based on the ideas of multiscale modeling facilitated by the VMS framework. The new stabilized method controls spurious oscillations in the advection dominated cases, effectively handles the Babuska-Brezzi (BB) inf-sup condition, accommodates arbitrary combinations of interpolation functions for the velocity and pressure fields, and yields a family of equal-order pressure-velocity elements [97].

### 3.3 The Variational Multiscale method

#### 3.3.1 Multiscale decomposition

The variational multiscale method [64, 65, 95] is based on an additive decomposition of the response functions into coarse and fine scales. The bounded domain $\Omega_t$ is discretized into sub-regions $\Omega_t^e$ (element domains) with boundaries $\Gamma_t^e$, $e = 1, 2, \ldots, n_e$, such that $\Omega_t = \bigcup_{e=1}^{n_e} \Omega_t^e$ and $\bigcap_{e=1}^{n_e} \Omega_t^e = \emptyset$, where $n_e$ denotes the number of elements in the discretized domain $\Omega_t$. We also define the union of element interiors as $\Omega' = \bigcup_{e=1}^{n_e} \text{int} \ \Omega_t^e$ and the union of element boundaries as $\Gamma' = \bigcup_{e=1}^{n_e} \Gamma_t^e$.

We assume an overlapping sum decomposition of the velocity field into coarse or resolvable scales and fine or sub-grid scales.
The fine-scale component \( v' \) is assumed to be represented by piecewise polynomials of sufficiently high order, continuous in space but discontinuous in time. In the present derivation, \( v' \) is assumed to be composed of piecewise constant-in-time functions. Accordingly, the time derivative of the velocity field is

\[
\frac{\partial v}{\partial t} = \frac{\partial \tilde{v}}{\partial t} \bigg|_{\tilde{y}} \quad (3.9)
\]

Likewise, we assume an overlapping sum decomposition of the weighting function into coarse and fine-scale components indicated as \( \tilde{w} \) and \( w' \), respectively:

\[
w(x) = \tilde{w}(x) + w'(x) \quad (3.10)
\]

We further make the assumption that the fine scales, although non-zero within the elements, vanish identically over the element boundaries.

\[
v_t' = w' = 0 \quad \text{on} \quad \Gamma' \quad (3.11)
\]

**Remark:** Stability and consistency of the method require that the spaces of functions for the coarse and fine scales are linearly independent. A comprehensive discussion on the topic is presented in [64, 65].

Substituting (3.8), (3.9) and (3.10) in the weak problem (3.6)-(3.7), we can decompose it into coarse-scale and fine-scale sub-problems.

**Coarse-scale sub-problem:**

\[
\left( \tilde{w}, \frac{\partial \tilde{v}}{\partial t} \right)_{\tilde{y}} + (\tilde{w}, (\tilde{v} + v' - v''') \cdot \nabla (\tilde{v} + v')) \\
+ (\nabla' \tilde{w}, 2v\nabla' (\tilde{v} + v')) - (\nabla \cdot \tilde{w}, p) - (\tilde{w}, f) - (\tilde{w}, h)_{\Gamma_h} = 0 \\
(q, \nabla \cdot (\tilde{v} + v')) = 0
\]  

(3.12)  

(3.13)
**Fine-scale sub-problem:**

\[
\begin{align*}
(w', \frac{\partial \bar{v}}{\partial t} |_y) + (w', (\bar{v} + v' - v^m) \cdot \nabla (\bar{v} + v')) \\
+ (\nabla' w', 2 \nu \nabla' (\bar{v} + v')) - (\nabla \cdot w', p) - (w', f) &= 0
\end{align*}
\]  

(3.14)

**Remark:** The key idea at this point is to solve the fine-scale sub-problem, defined over the sum of element interiors, to obtain the fine-scale solution in terms of the coarse-scale residual. This solution is then substituted in the coarse-scale sub-problem thereby eliminating the explicit appearance of the fine scales. This step introduces additional terms in the coarse-variational form, called the stabilization terms.

### 3.3.2 Solution of the fine-scale sub-problem

Let us consider the fine-scale sub-problem (3.14). Our objective is to solve this sub-problem so as to get a closed-form expression for the fine-scale velocity field in terms of the coarse-scale residuals. Since (3.14) is a non-linear problem with respect to \( v' \), the problem needs to be simplified so that a closed-form expression for the fine-scale solution \( v' \) can be developed. This can be considered as the modeling part in the proposed method.

We consider (3.14) and keep all the terms that contain \( v' \) on the left hand side of the equation and move the remaining terms to the right hand side. The resulting equation is

\[
\begin{align*}
(w', v' \cdot \nabla \bar{v}) + (w', (\bar{v} - v^m) \cdot \nabla v') + (w', v' \cdot \nabla v') + (\nabla' w', 2 \nu \nabla' v') = \\
-(w', \frac{\partial \bar{v}}{\partial t} |_y) - (w', (\bar{v} - v^m) \cdot \nabla \bar{v}) - (\nabla' w', 2 \nu \nabla' \bar{v}) + (\nabla \cdot w', p) + (w', f)
\end{align*}
\]  

(3.15)

Integrating by parts the viscous and pressure terms that are on the right hand side of (3.15) and using the fact that \( w' \) vanishes on the boundaries of the elements as presented in (3.11), the fine-scale sub-problem reads as

\[
\begin{align*}
(w', v' \cdot \nabla \bar{v}) + (w', (\bar{v} - v^m) \cdot \nabla v') + (w', v' \cdot \nabla v') + (\nabla' w', 2 \nu \nabla' v') = \\
+ (\nabla' w', 2 \nu \nabla' v') = -(w', r)
\end{align*}
\]  

(3.16)

where \( r \) is the residual of the Euler-Lagrange equations defined as follows:

\[
r = \frac{\partial \bar{v}}{\partial t} |_y + (\bar{v} - v^m) \cdot \nabla \bar{v} - 2 \nu \Delta \bar{v} + \nabla p - f
\]  

(3.17)
Considering that the sub-grid solution $v'$ is usually a small perturbation to the total solution, we drop the higher-order term $(w', v' \cdot \nabla v')$ in order to simplify the fine-scale sub-problem. This makes the fine-scale sub-problem linear with respect to $v'$. Assuming that the fine scales $v'$ and $w'$ are represented via bubble functions $b^e(\xi)$ over $\Omega'$ (i.e., $v' = \beta b^e(\xi)$ and $w' = \gamma b^e(\xi)$), the fine-scale solution is expressed as

$$v'(x) = -b^e \left[ \int (b^e)^2 \nabla^T \nu \, d\Omega + \int b^e (\bar{v} - v^m) \cdot \nabla b^e \, d\Omega \right]^{-1} \int b^e r \, d\Omega$$

(3.18)

In order to further simplify the expression for the fine-scale solution, we assume that the residual $r$ is piecewise constant over the element interiors. This results in a projection of the fine-scale solution onto the coarse-scale basis, wherein the projector captures the mean value of the residual over the element interiors. The resulting fine-scale solution is

$$v'(x) = -\tau r$$

(3.19)

where the stabilization tensor $\tau$ is defined as

$$\tau = b^e \int b^e \, d\Omega \left[ \int (b^e)^2 \nabla^T \nu \, d\Omega + \int b^e (\bar{v} - v^m) \cdot \nabla b^e \, d\Omega \right]^{-1} \int \nabla b^e \otimes \nabla b^e \, d\Omega$$

(3.20)

Remark: Technical discussion on appropriate bubble functions needed to solve the fine-scale sub-problem can be found in [97]. A simple procedure for the design of bubble functions that can yield the desired behavior of the stabilization tensor $\tau$ can be found in [96].

Remark: One way of solving the nonlinear fine-scale problem is to perform consistent linearization of the fine-scale problem, as was advocated in [97]. Consistent linearization in the present context would also lead to the same definition of $\tau$ as the one given in (3.20).

Remark: Approaches that are based on developing approximations to the element Green’s function problem have been used extensively in the literature. Interested reader is directed to Bazilevs et al. [10] and references therein.
3.3.3 Solution of the coarse-scale sub-problem. The nonlinear stabilized form

Let us now consider the coarse-scale problem (3.12)-(3.13). Equation (3.12) can be expanded as

\[
\left( \frac{\partial \vec{F}}{\partial t} \right)_y + (\vec{w},(\vec{v} - \nu^m) \cdot \nabla \vec{v}) + (\vec{w},(\vec{v} - \nu^m) \cdot \nabla \nu') \\
+ (\vec{w},\nu' \cdot \nabla \vec{v}) + (\vec{w},\nu' \cdot \nabla \nu') + (\nabla' \vec{w}, 2\nu \nabla' \vec{v}) \\
+ (\nabla' \vec{w}, 2\nu \nabla' \nu') - (\nabla \cdot \vec{w}, p) - (\vec{w}, f) - (\vec{w}, h)_{\tau_h} = 0
\]  

(3.21)

There are four convective terms in (3.21). The first term \((\vec{w},(\vec{v} - \nu^m) \cdot \nabla \vec{v})\) is the classical convective term for the coarse scales. The next two terms, \((\vec{w},(\vec{v} - \nu^m) \cdot \nabla \nu')\) and \((\vec{w},\nu' \cdot \nabla \vec{v})\), are called the cross-terms. The last term \((\vec{w},\nu' \cdot \nabla \nu')\) is a higher-order term and is usually called the fine-fine term. As done earlier for the fine-scale sub-problem, we neglect this higher order-term. Employing integration by parts on the terms that involve derivatives of \(\nu'\), and using the fact that fine scales vanish on the boundaries of the elements, (3.21) can be written as

\[
\left( \frac{\partial \vec{F}}{\partial t} \right)_y + (\vec{w},(\vec{v} - \nu^m) \cdot \nabla \vec{v}) + (\nabla' \vec{w}, 2\nu \nabla' \nu') \\
- (\vec{w} \nabla \cdot (\vec{v} - \nu^m) + (\vec{v} - \nu^m) \cdot \nabla \vec{w} - \vec{w} \cdot \nabla^T \vec{v} + 2\nu \Delta' \vec{w}, \nu') \\
- (\nabla \cdot \vec{w}, p) - (\vec{w}, f) - (\vec{w}, h)_{\tau_h} = 0
\]  

(3.22)

Likewise, considering the continuity equation (3.13), and integrating by parts the fine-scale term we get

\[(q, \nabla \cdot \vec{v}) - (q \cdot \nu', \nu') = 0\]  

(3.23)

We now combine (3.22) and (3.23), and substituting the fine-scale solution (3.19) to the resulting equation we get the final stabilized form

\[
\left( \frac{\partial \vec{F}}{\partial t} \right)_y + (\vec{w},(\vec{v} - \nu^m) \cdot \nabla \vec{v}) + (\nabla' \vec{w}, 2\nu \nabla' \nu') - (\nabla \cdot \vec{w}, p) + (q, \nabla \cdot \vec{v}) \\
+ (\vec{w} \nabla \cdot (\vec{v} - \nu^m) + (\vec{v} - \nu^m) \cdot \nabla \vec{w} - \vec{w} \cdot \nabla^T \vec{v} + 2\nu \Delta' \vec{w} + \nabla q, \tau r) \\
= (\vec{w}, f) + (\vec{w}, h)_{\tau_h}
\]  

(3.24)

In equation (3.24) the first five terms on the left hand side and the terms on the right hand side are the standard Galerkin terms. The sixth term, which arises because of the
projection of the fine scales onto the coarse-scale space, leads to the stabilization terms. It is important to note that stabilization terms contain a term which is proportional to the divergence of the difference of the particle and the mesh velocity. Even though fluid velocity is almost divergence-free, the divergence of the mesh velocity may be arbitrarily large and can be either positive or negative. This issue was studied in Masud [91] and it was shown that the condition of divergence-free relative velocity serves as a form of the Geometric Conservation Law (GCL) for the advection-diffusion equation when written in an ALE framework. This has two important implications:

(i) The mesh motion schemes need to satisfy the internal constraint of divergence-free motion of the mesh that may not always be possible for large amplitude motions, and

(ii) Even when this condition imposed by GCL is satisfied, the constant in the bound on the error norm for the advection dominated case becomes a function of the semi-norm of the relative mesh velocity.

Consequently, there still exists a potential cause of instability due to the dependence of the constant on the spatial grid velocity that can be arbitrarily large.

Remark: The fine-fine term, \((\vec{w}, \nabla \cdot \nabla ')\), which has been neglected in the present formulation, is a crucial term in the modeling of turbulence within the context of the variational multiscale method [10].

Remark: If we consider the Eulerian limit of the formulation (i.e., \(v^m = 0\)) the formulation presented in [97] is recovered.

Remark: If the Lagrangian limit of the formulation is considered (i.e., \(v^m = v\)) then as expected all the standard convective terms disappear [109]. However, term \((\vec{w} \cdot \nabla ^T \vec{v}, \tau r)\) in equation (3.24), and term \(\int (b^e)^2 \nabla ^T \vec{v} d\Omega\) in the definition of the stabilization parameter (3.20) do not vanish despite the fact that they are also convective terms.
Remark: It is important to realize that in stabilized formulations for transient problems, the consistent mass contains additional terms that appear due to the appearance of time-derivative terms in the stabilization. Accounting for these terms is important for temporal accuracy.

3.4 The mesh moving technique

To simulate flows with moving domains using the ALE framework, two key ingredients are needed. The first one is a formulation written in the ALE framework which was presented in Section 3.3. The second ingredient is a technique to move the boundaries of the fluid domain and therefore of the computational grid that is used to discretize it. In this work we employ the mesh moving technique that was developed by the senior author and his co-workers and is presented in [86, 94, 75]. This mesh moving technique has common roots with the one introduced in [127, 72].

Let us consider the time-dependent fluid domain $\Omega_t$. For mesh moving problems the domain boundary $\Gamma_t$ can be decomposed into a portion that is fix and therefore does not deform ($\Gamma^f_t$), and a portion that deforms to represent the evolving fluid domain ($\Gamma^m_t$). For uniqueness, this new decomposition of the domain boundary is required to satisfy the conditions $\Gamma = \Gamma^f \cup \Gamma^m_t$ and $\Gamma^f \cap \Gamma^m_t = \emptyset$.

Given the prescribed displacement field $g(x, t)$ at the moving portion of the boundary $\Gamma^m_t$, the displacement field for the computational grid is evaluated by the following modified Laplace equation

$$\nabla \cdot \left( [1 + \alpha^e] \nabla u \right) = 0 \quad \text{in } \Omega_t \quad (3.25)$$

$$u = g(x, t) \quad \text{on } \Gamma^m_t \quad (3.26)$$

$$u = 0 \quad \text{on } \Gamma^f \quad (3.27)$$

where the parameter $\alpha^e$ is function of the local element size and is defined as follows:

$$\alpha^e = \frac{1 - V_{\min}/V_{\max}}{V_e/V_{\max}} \quad (3.28)$$
where $V_e$ is the volume of element $e$ and $V_{\text{min}}$ and $V_{\text{max}}$ are the volumes of the smallest and largest elements in the mesh, respectively. Figure 3.1 shows graphical representation of $\alpha^e$ given in (28) as a function of the volume of elements in a generic mesh.

The parameter $\alpha^e$ controls the relative distortion of elements in the mesh. Smaller elements are selectively made stiffer as compared to the larger elements in the mesh that usually lie away from the boundary layer regions. Thus, smaller elements translate with the moving boundary with the least amount of distortion and the larger elements being relatively soft, absorb the significant part of the deformation of the mesh. Similar effects can be attained using the technique presented in [127, 72, 73].

### 3.5 Numerical results

This section presents numerical results obtained with the proposed method and shows its validity and range of applicability. In all these simulations we have employed equal-order pressure-velocity elements using linear hexahedral shape functions. Time discretization is done via the Backward Difference Formula (BDF2) scheme, which is a second order accurate scheme. In the evaluation of the element level integrals, standard Gauss integration rules are used. In addition, standard quadratic bubble functions are employed to compute the stabilization parameter $\tau$. In order to preserve the skew part in $\tau$ we follow the procedure presented in our earlier works [89, 92, 97] and employ a different order bubble in the weighting function slot corresponding to the advection term. This also helps in bringing in an up-winding effect in the computed stabilization parameter.

The first test case is that of transient vortex shedding around a fixed cylinder which is a standard benchmark problem to check the stability and accuracy of numerical methods. The next three test cases involve moving fluid-solid boundaries. The first of these test cases is that of vortex shedding from a cylinder which is held in place in the transverse direction by attaching it to a linear spring, while it is constrained to move in the mean stream-wise direction. Thus, the cylinder moves in the transverse direction due to the lateral forces produced by the periodic vortices. The second simulation models the flow field around a beam that is oscillating with a given motion. In all the test cases presented so far, the fluid flow is kept two-dimensional by having only one layer of elements through the thickness
direction. The last test case simulates three-dimensional effects. In particular, a cylinder is again attached to a linear spring and full three-dimensional flow features are allowed to develop.

3.5.1 Vortex shedding around a fix cylinder

Modeling of flow field around a circular cylinder is a classical benchmark problem that is used to assess the accuracy of numerical methods that are based on transient Navier-Stokes equations [13]. The physical problem consists of a cylinder that is fix in space and is surrounded by flowing fluid. As the flow develops, the boundary layer detaches from the cylinder and gives rise to two dominant vortices behind the cylinder. As the Reynolds number gets sufficiently high, usually considered \( \text{Re} \geq 40-45 \), these vortices are convected downstream of the cylinder and new vortices are formed behind the cylinder in a periodic fashion. Typically, the numerical accuracy of the formulation for simulations of this problem is checked by means of the Strouhal number (inverse of the period in which vortices are detached from the cylinder).

Figure 3.2 shows a schematic diagram of this problem. For comparison purposes, we have used the same problem description, dimension, and spatial discretization as the one used in Hauke and Hughes [53]. The viscosity \( \nu \) of the fluid is 0.01. The velocity field on the inflow boundary is set equal to 1. No-slip boundary condition is prescribed on the surface of the cylinder to account for the viscous adhesion, and traction-free conditions are imposed on the outflow boundary. Zero normal velocity and zero shear stress conditions are prescribed on the remaining boundaries of the computational domain. The flow is initially at rest and the inflow velocity is gradually increased until it reaches \( v_x = 1 \). Reynolds number based on the inflow velocity and the diameter of the cylinder is 100. The computational domain is discretized with one layer of 4,936 hexahedral elements. The time step \( \Delta t \) is set equal to 0.01.

Figure 3.3 shows the stationary streamlines and the velocity field at a given time level when the flow is fully developed. Flow field generates viscous and pressure forces that act on the surface of the cylinder. We define the lift coefficient as \( C_L = F_y / 0.5 \rho v_x^2 D H \), where \( F_y \) is the force acting on the cylinder in the transverse direction, \( \rho = 1 \) is the density, \( v_x = 1 \) is the input velocity, \( D = 1 \) is the diameter of the cylinder and \( H = 0.05 \) is its height.
Likewise, we define the drag coefficient as \( C_D = \frac{F_x}{0.5 \rho v_s^2 D H} \), where \( F_x \) is the force acting on the cylinder along the mean-stream direction. The evolution of the lift and drag coefficients is shown in Figs. 3.4(a) and 3.4(b), respectively.

The period of vortex shedding \( T \) can be calculated from the time-plot of the lift coefficient. The computed period is 5.7 and the corresponding Strouhal number (\( St = 1/T \)) is 0.175. Similar results for this problem have been reported in Hauke and Hughes [53], wherein using time step \( \Delta t = 0.025 \) they obtained \( St = 0.172 \). Strouhal numbers obtained in our study and in [53] are higher than the experimentally obtained Strouhal number, which is 0.167. One of the reviewers pointed out that Tezduyar and his associates in [13] attributed such discrepancies to the close proximity of the lateral boundaries. Their study concluded that in order to get a solution that is independent of the location of the boundaries, these should be placed at least 12 diameters away from the cylinder. Accordingly, we repeated the simulation with the lateral boundaries located at 12 diameters away from the center of the cylinder. With the new spatial domain we obtain \( St = 0.167 \), which coincides with the Strouhal number reported in [13]. The corresponding lift and drag coefficients are presented in Figures 3.5(a) and 3.5(b), respectively.

### 3.5.2 Vortex shedding around a cylinder attached to a linear spring

This problem is an extension of the one studied in Sec. 3.5.1. We again consider a cylinder of unit diameter that is fix in the stream-wise direction. However, in the present case the displacement of the cylinder in the direction normal to the stream-wise direction is constrained by a linear spring. This problem was extensively studied in [101]. The fluid forces acting on the cylinder move the cylinder in the transversal direction while the reaction force that develops in the spring tries to pull it back to its equilibrium state. Other characteristics of the problem are kept same as in the problem studied in Sec. 3.5.1, i.e., the spatial description of the problem is similar to the one sketched in Fig. 3.2. Since the lateral boundaries are at six diameters from the center of the cylinder, we anticipate that the computed solution will have some effect that is induced due to the close proximity of the lateral boundaries. In this simulation, time step is \( \Delta t = 0.025 \).

The mass of the cylinder is \( M = 8.23 \times 10^{-2} \) and the stiffness of the linear spring is \( K = 0.1 \). This choice leads to the natural period of this spring-mass system
Recall that for the case of the fix cylinder in Sec. 3.5.1 the period of vortex shedding is also $5.7$. Accordingly, it is a model problem for a strongly coupled fluid-structure system with synchronization or lock-in of the vortex-shedding frequency to the oscillation frequency of the structure. The structure is a rigid body with just one degree of freedom given by the following equation

$$M \frac{d^2 y}{dt^2} + C \frac{dy}{dt} + Ky = F_f$$

(3.29)

where $y$ is the displacement of the cylinder, $F_f$ is the unsteady lift force induced by the fluid and $C$ is the damping coefficient, which has been assumed to be zero in all the cases considered here.

The coupled iterative solution scheme is briefly described below:

(i) At a given time level, the location of the equilibrated state of the cylinder is calculated via (29) and the configuration of the spatial mesh is appropriately updated.

(ii) The fluid equations are solved in the updated fluid domain.

(iii) If compatibility conditions between the fluid and the cylinder are satisfied, the algorithm moves on to the next time level. Else, steps 1, 2 and 3 are repeated.

As the flow develops, the time-dependent lift force that acts on the cylinder starts oscillating the cylinder about its equilibrium position. After an initial transient regime, the problem reaches a periodic state wherein the period of oscillation is $T = 5.94$. This yields a Strouhal number $St = 0.168$. Analyzing the evolution of the displacement of the cylinder we see that the maximum amplitude of oscillation is 0.48. The evolution of the displacement of the cylinder is presented in Fig. 3.6(a), the phase diagram between the lift coefficient and the displacement of the cylinder in the periodic state is shown in Fig. 3.6(b), and the evolution of lift and drag coefficients is shown in Fig. 3.7(a-b).

Figure 3.8 shows the stationary streamlines and the velocity field at a given time level when the flow is fully developed. The pattern of the streamlines in the present case is clearly different from the one obtained for the case of the fix cylinder (see Fig. 3.3).
A simple \textit{a priori} analysis of the problem would have lead one to conclude that since the natural period of the spring-mass system is the same as that in the transient vortex shedding problem, the two are strongly coupled and the spring-mass system is in resonance. However, the current numerical study that takes into account the coupling between the fluid flow and the cylinder reveals that the fully coupled system is stable and periodic.

\textbf{Remark:} A time step-size study was also carried out to check the accuracy of the numerical method. For a smaller time step, $\Delta t = 0.01$, the amplitude and period of the displacement of the cylinder were also found to be $A = 0.48$ and $T = 5.94$, respectively.

\textbf{Remark:} The global Reynolds number based on the input velocity and the diameter of the cylinder is 100. A local Reynolds number based on the maximum velocity of the cylinder can also be defined and in the present simulation this local Reynolds number is 51. However, for other parameters of the coupled fluid-structure system the local Re can be much higher than the global Re. In that case the spatial and temporal discretization of the domain around the cylinder needs to be refined in order to maintain the overall accuracy of the solution.

3.5.3 \textbf{Flow around a deforming beam}

In this section we consider an elastic beam that is fixed in a square base and is undergoing large amplitude oscillations with a prescribed displacement field. The geometric parameters are similar to the ones used in Wall and Ramm [132] wherein full elastic interactions are also considered.

Figure 3.9 presents a schematic description of the problem. The beam is stationary for $0 < t \leq 2$. For $t > 2$, the transverse displacement of the beam is given by

$$g_y(x, t) = A (x - 0.5)^2 \sin \left( \frac{2\pi}{T} (t - 2) \right)$$  \hspace{1cm} (3.30)$$

where $A = 0.075$ and the period of the motion is $T = 10$. The variable $x$ refers to the axial location of a material point in the un-deformed configuration. In order to maintain the length of the beam during large amplitude oscillations, a non-zero displacement in the $x$ direction is also prescribed:

$$g_x(x, t) = -C g_y(x, t) \tan(\theta(x, t)) - y \sin(\theta(x, t))$$  \hspace{1cm} (3.31)$$
where $\theta(x,t)$ is the instantaneous angle between the beam and the $x$-direction and $C = 0.25$ is a parameter chosen so that the length of the beam is approximately conserved.

On the inflow boundary $v_x = 1$ is imposed, while on the outflow boundary the zero-traction condition is prescribed. No-slip condition is prescribed on the surface of the beam to account for viscous adhesion. Zero normal velocity and zero shear stress are prescribed on the remaining parts of the boundaries. The computational domain is discretized with one layer of 6807 hexahedral elements. Time step $\Delta t$ is set equal to 0.025.

Figure 3.10 shows the deformed shape of the beam at $t = 20.0$, which corresponds to an instant when the beam is moving upwards. This figure also shows the pressure field at the same time level. Since the beam is pushing the fluid upwards, the pressure above the beam is higher than that in the region below the beam.

The time history of pressure at the middle of the beam is plotted in Fig. 3.11. When the flow reaches a periodic state, the lag between the evolution of the pressure field on the top and the bottom surface is $T/2 = 5$. Figure 3.12 shows the pressure profile along the top surface of the beam at two different time levels. Figure 3.13 presents the evolution of the velocity field at a point that is downstream of the beam (i.e., $(x,y) = (7,0)$). This figure shows that for $t > 25$ the solution reaches a periodic state.

### 3.5.4 3D flow around a cylinder attached to a linear spring

The problem considered in this section is a 3D extension of the problem studied in Sec. 5.2, wherein the simulated flow field around the cylinder is at $Re = 100$. In 3D configurations the flow can develop full 3D features when $Re > 180$.

The spatial $x$-$y$ dimensions of the computational domain are similar to the one in Fig. 3.2. In the present case, the depth along the direction of the axis of the cylinder is 5. The displacement of the cylinder in the stream-wise direction is restrained, and in the transversal direction the cylinder is attached to a linear spring. A unit velocity is prescribed on the inflow ($v_x = 1$), traction-free condition is imposed on the outflow, no-slip condition is prescribed on the surface of the cylinder, and zero normal velocity and zero shear stress are prescribed on the remaining parts of the boundary.
The viscosity of the fluid is \( \nu = 0.00333 \). Based on the inflow velocity and the diameter of the cylinder, the Reynolds number is 300. For this Reynolds number, Kalro and Tezduyar [74] have reported that the period of vortex shedding from a corresponding fixed cylinder is \( T = 4.93 \) (St = 0.203). We choose a stiffness for the spring and a mass for the cylinder such that the natural period of the spring-mass system is \( T_N = 4.93 \). In particular we choose \( K = 10 \) and \( M = 5.13 \). Accordingly, the vortex-shedding frequency is synchronized with the oscillation frequency of the structure. The three-dimensional domain is discretized with 40 layers of elements wherein each layer consists of 4,936 hexahedral elements. Consequently the mesh has 197,440 elements and the total number of degrees of freedom is 810,080. The time step \( \Delta t \) is set equal to 0.05.

Figure 3.14(a) shows the evolution of the displacement field of the cylinder in the transverse direction to the mean flow. The phase plot between the displacement of the cylinder and the lift coefficient, obtained with \( \Delta t = 0.025 \), is presented in Fig. 3.14(b). Like the 2D case, the displacement of the cylinder attains a periodic state in the 3D case as well. The computed period is \( T = 4.58 \) (St = 0.218) and the amplitude of oscillation is 0.52. Since the lateral boundaries are at six diameters from the center of the cylinder, the computed amplitude may have some effects that are induced due to the close proximity of the lateral boundaries. Figure 3.15(a-b) shows the evolution of the lift and drag coefficients. Figure 3.16 shows the velocity field and some significant stationary streamlines at \( t = 50.3 \) and \( t = 52.6 \). Additionally, three dimensional structures of the flow are shown via iso-surfaces of the span-wise component of the velocity field.

### 3.6 Conclusions

We have presented a variational multiscale (VMS) based stabilized method for the incompressible Navier-Stokes equations. The new method is developed in ALE framework to model fluid flow problems with moving boundaries and fluid-solid interfaces. The VMS framework facilitates the decomposition of the variational problem into two sub-problems, thus leading to the sub-grid scale modeling concept. In the proposed method the fine-scale sub-problem is solved via bubble functions, and this approach enables the derivation of the stabilization tensor directly from the fine-scale sub-problem. An attribute of the VMS based stabilized methods for the Navier-Stokes equations is that higher-order terms arise in both the
fine-scale and the coarse-scale sub-problems. These higher-order terms and especially the ones that are associated with the coarse-scale sub-problem are crucial in the modeling of turbulence phenomena. However, these higher-order terms are not significant in laminar flows and are therefore not considered in the present implementation. The new ALE formulation is consistent with the Eulerian formulation presented in our earlier work [97], where a stabilized method was derived for problems with fix boundaries. Several numerical simulations are presented that show the good stability and accuracy properties of the new method.

3.7 Figures

**Figure 3.1** Parameter $\alpha^e$ as a function of the relative volume of the elements

**Figure 3.2** Schematic diagram of the vortex-shedding problem
Figure 3.3 Fix cylinder. Stationary streamlines superposed on the resultant velocity field

Figure 3.4 Fix cylinder. Evolution of the (a) lift and (b) drag coefficients
Figure 3.5 Fix cylinder in a larger domain. Evolution of the (a) lift and (b) drag coefficients
Figure 3.6 Cylinder attached to a linear spring. (a) Evolution of the transversal displacement of the cylinder, and (b) Lift coefficient versus the displacement of the cylinder in the periodic state regime.
Figure 3.7 Cylinder attached to a linear spring. Evolution of the (a) lift and (b) drag coefficients

Figure 3.8 Cylinder attached to a linear spring. Stationary streamlines superposed on the resultant velocity field
Figure 3.9 Schematic diagram of the deforming beam problem

Figure 3.10 Pressure field at t = 20
Figure 3.11 Evolution of the pressure field at the middle of the beam

Figure 3.12 Pressure field at the top surface of the beam at $t = 22$ and $t = 27$

Figure 3.13 Evolution of the velocity field of the fluid downstream of the beam ($x = 7$, $y = 0$)
Figure 3.14 (a) Evolution of the displacement of the 3D cylinder, and (b) lift coefficient versus the displacement in the periodic state regime.
Figure 3.15 Evolution of the (a) lift, and (b) drag coefficients for the 3D cylinder problem
Figure 3.16 Velocity field superposed onto spanwise velocity iso-surfaces and streamlines at (a) $t = 50.3$, and (b) $t = 52.6$. This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.
Chapter 4

A Variational Multiscale method for incompressible turbulent flows: Bubble functions and fine scale fields*

4.1 Motivation

Large Eddy Simulation (LES) provides computationally economic solutions to the modeling of turbulence as compared to the Direct Numerical Simulation (DNS) wherein all the scales of turbulence are numerically resolved. Several techniques have been adopted under the traditional LES framework to model the small scale effects in the turbulent flow regime and reasonable success has been achieved for various geometric configurations and Reynolds numbers. Most of the traditional LES techniques emphasize the use of eddy viscosity models such as the constant-coefficient Smagorinsky-type models [118] and the dynamic viscosity models [44, 81]. Nevertheless, LES models that are not based on viscosity models have also been proposed [92]. For a non-exhaustive collection of methods for LES modeling, the reader could refer to [118, 9, 44, 81, 29, 68, 102, 85, 105, 122, 135] and references therein.

In recent years new LES models that are based on the Variational Multiscale (VMS) framework proposed by Hughes et al. [64, 65] have been presented. The first applications of the VMS method to the modeling of turbulence by Hughes et al. [66, 67] were based on three-level scale decomposition involving coarse-, fine- and the modeled-scales. The early versions of VMS-based turbulence models employed both Smagorinsky-type constant-coefficient viscosities [118], as well as the dynamic viscosities [44, 81], and good results were obtained for a variety of test cases. It was observed that within the VMS framework, the dynamic viscosity models yield superior results as compared to the static eddy viscosity models.

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Adopting VMS approach, three-scale turbulence models in the context of finite element methods were presented in [26, 47, 48], and in the context of finite volume methods on unstructured grids were presented by Farhat and co-workers [78, 35, 116, 117].

Subsequent developments in VMS based turbulence models adopted a two-level scale separation [106, 10, 25, 2, 11, 43, 55]. The key idea underlying the VMS framework is a-priori direct sum decomposition of the space of functions into coarse- and fine-scale space. This decoupling of the physical scales that is manifested via the appropriate spaces of functions is linked to a decomposition of the computational scales into two overlapping components that are categorized as coarse-scales and fine-scales, respectively. Typically the coarse-scales are represented via the traditional finite element shape functions, while the fine-scales that lie in an infinite-dimensional space, are defined to be the remaining part of the solution. The decoupling of the spaces of functions leads to the decomposition of the original problem into two sub-problems, namely, the coarse-scale sub-problem and the fine-scale sub-problem. The modeling aspect in the method lies in extracting the fine-scale solution from the nonlinear fine-scale sub-problem. This fine-scale solution is then variationally projected onto the coarse-scale space, leading to a formulation that is expressed entirely in terms of the coarse-scales. This contribution of the nonlinear fine-scales that leads to nonlinear stabilization is interpreted as a way to model the turbulence phenomena. Although the final formulation does not depend explicitly on the fine-scale fields, the effects of fine-scales are consistently represented via the additional residual based terms. The large scale features in the solution of the final form are computationally resolved, and this aspect of the VMS-based models shares common threads with the LES strategies.

In this Chapter we primarily focus our attention to the modeling of the nonlinear fine-scale problem. Since the fine-scale velocity lies in an infinite-dimensional space, as a consequence, the fine-scale problem cannot be exactly resolved. This requires modeling assumptions on the fine-scales to help reduce the dimensionality of the problem and to estimate the fine-scale features that can then be projected onto the coarse-scale space. We endeavor to extend our earlier work on the variational multiscale methods in the context of laminar flows [97, 20] wherein fine-scale problem was expanded in terms of bubble functions, to residual based turbulence models. The use of bubble functions for the modeling of fine-scales was successfully applied by us in the derivation of stabilized formulations for a variety
of mixed field problems [89, 90, 92, 77, 93, 96]. In this Chapter we show that in the context of turbulent flows, the use of bubble functions for expanding fine-scales leads to various design options for the VMS based turbulence models. The effects of these options on the numerical solution of the coarse-scale problem are investigated in the numerical section.

The Chapter is organized as follows. In Sec. 4.2 the incompressible Navier-Stokes equations are presented. In Sec. 4.3 we present the derivation of the residual-based turbulence model, where the time-dependent aspects of the fine-scales are emphasized. In Sec. 4.4, the proposed method is studied numerically via three test cases with increasing degree of complexity in the flow physics. In Sec. 4.4.2, using the turbulent channel flow problem for two different Re flows, we investigate the computational attributes of the various modeling assumptions stipulated in Sec. 4.3. Specifically, we evaluate the effects of fine-scale pressure field that is manifested via an element-wise continuity term. We study the effects of accounting for the orthogonality of the sub-grid scales to the coarse-scale space that leads to the annihilation of the sub-grid scale viscosity term, and compare it with the case when this condition is not imposed. An important aspect of the fine-scale modeling involved in the fine-scale problem is the consideration and numerical evaluation of the residual of the Euler-Lagrange equations of the coarse-scales. We investigate the influence of considering the mean value of the residual versus the full residual on the modeled fine-scale velocity field in an effort to develop a mathematically rigorous and computationally economic model. An important issue in the modeling of reactive turbulent flows is that of the time step size in the otherwise implicit time integration schemes. It is now well documented that if the step-size employed in implicit schemes is of the order of the step-size of its underlying explicit-in-time scheme, spurious oscillations can appear [51]. This aspect is attributed to the issue of the violation of the principle of causality. In Sec. 4.4.2.5 we show that if the time terms in the expansion of the fine-scale velocity field are fully accounted for in the fine-scale time integration, this issue can be adequately addressed. Conclusions are drawn in Sec. 4.5.

4.2 The incompressible Navier-Stokes equations

Let $\Omega \subset \mathbb{R}^{n_{sd}}$ be a connected, open, bounded region with piecewise smooth boundary $\Gamma$. The number of space dimensions, $n_{sd}$, is equal to 3. The time interval of interest is
denoted \( \mathbb{T} \), with \( T > 0 \). The initial/boundary-value problem consists of solving the following set of equations for \( v : \Omega \times \mathbb{T} \rightarrow \mathbb{R}^{n_d} \), the velocity, and \( p : \Omega \times \mathbb{T} \rightarrow \mathbb{R} \), the kinematic pressure:

\[
\begin{align*}
\frac{\partial v}{\partial t} + \nabla \cdot (v \otimes v) - 2\nu \nabla \cdot v + \nabla p &= f \quad \text{in } \Omega \\
\nabla \cdot v &= 0 \quad \text{in } \Omega \\
v &= g \quad \text{on } \Gamma \\
v(x,0) &= v_0 \quad \text{on } \Omega
\end{align*}
\] (4.1)

where \( f : \Omega \times \mathbb{T} \rightarrow \mathbb{R}^{n_d} \) is the body force (per unit of mass), \( v \) is the kinematic viscosity (assumed positive and constant), \( v_0 \) is the initial condition for the velocity field, \( g \) represents the Dirichlet boundary conditions, and \( \otimes \) denotes the tensor product. \( \varepsilon(v) \) is the strain-rate tensor which is defined as \( \varepsilon(v) = \nabla v = \left[ \nabla v + (\nabla v)^T \right]/2 \). Equation (4.1) is the momentum balance equation; equation (4.2) is the incompressibility constraint; equations (4.3) is the Dirichlet boundary condition; and (4.4) is the initial condition.

Let \( w(x) \in V = \left( H^1_0(\Omega) \right)^{n_d} \) and \( q(x) \in Q = C^0(\Omega) \cap L^2(\Omega) \) represent the weighting functions for the velocity and the pressure fields, respectively. The appropriate spaces of functions for the velocity and pressure trial solutions are the corresponding time-dependent spaces \( \mathcal{S} \) and \( \mathcal{P} \) that satisfy the initial and boundary conditions \textit{ab-initio}. The standard weak form of the problem is: find \( v(x,t) \in \mathcal{S} \) and \( p(x,t) \in \mathcal{P} \) such that for all \( w(x) \in V \) and \( q(x) \in Q \),

\[
\begin{align*}
(w, \frac{\partial v}{\partial t}) - (\nabla w, v \otimes v) + (\nabla' w, 2\nu \nabla' v) - (\nabla \cdot w, p) &= (w, f) \\
(q, \nabla \cdot v) &= 0
\end{align*}
\] (4.5)

(4.6)

where \((\cdot, \cdot) = \int_{\Omega} \left( \cdot, \cdot \right) d\Omega \) is the \( L^2(\Omega) \)-inner product. Equations (4.5) and (4.6) imply weak satisfaction of the momentum equations and the continuity equation, in addition to the initial condition.
Remark: For the derivation of the VMS method presented in Section 4.3, we consider only the Dirichlet boundary conditions.

4.3 The Variational Multiscale method

Let \( \{ \Omega^e \}_{e=1}^{n_{el}} \) be a partition of \( \Omega \) such that \( \bigcup_{e=1}^{n_{el}} \Omega^e = \Omega \) and \( \bigcap_{e=1}^{n_{el}} \Omega^e = \emptyset \). Here \( n_{el} \) denotes the number of elements in the domain \( \Omega \). The boundaries of the elements \( \Omega^e \) are \( \Gamma^e \), \( e = 1, 2, \ldots, n_{el} \). The variational multiscale method [64, 65, 95] consists of decomposing the velocity field and the weighting functions into coarse- and fine-scales. The coarse-scale field belongs to a finite dimensional space of functions, and is typically represented by finite element shape functions. The fine-scale field, also called sub-grid scale field, is the remaining part of the solution. Although the space of the fine-scale field is infinite dimensional, it will be approximated by a finite dimensional sub-space spanned by the bubble functions and this will constitute the modeling part of the fine-scale problem.

We assume a unique additive decomposition of the velocity field into coarse, or resolvable scales \( \bar{v} \), and fine, or un-resolvable scales \( v' \) that are also considered as the rapidly fluctuating part of \( v \):

\[
v(x,t) = \bar{v}(x,t) + v'(x,t)
\]  

(4.7)

The coarse and fine-scale fields belong to spaces of functions that accommodate a direct sum decomposition into \( \bar{S} \) and \( S' \), respectively.

\[
\mathcal{S} = \bar{S} \oplus S'
\]  

(4.8)

\[
S' = \mathcal{S} \setminus \bar{S}
\]  

(4.9)

where \( \bar{S} \) is a finite-dimensional space typically identified with the standard finite element space (defined in Section 4.2). The fine-scale space \( S' \) is infinite dimensional and therefore various characterizations of \( S' \) are possible for the approximation of the fine-scale velocity field \( v' \) (see, e.g., [64]).

Remark: In our previous works [97, 20], the fine-scale component \( v' \) was assumed to be represented by piecewise polynomials of sufficiently high order, continuous in space but
piecewise constant-in-time. In this Chapter we relax the later assumption and allow the fine scales to continuously evolve in time.

**Remark:** Time dependent fine-scales are important to resolve some issues that appear when very small time step sizes are employed. For example, in residual-based turbulence models, for the case of quasi-static fine-scales, the fine-scale velocity field vanishes as the size of the time step approaches zero. In addition, time dependent fine-scales are important to resolve the issues that are encountered when a very small step-size is employed in implicit time integration methods [51]. Residual-based turbulence models that consider the time-dependence of fine-scales have also been proposed in [43, 55].

Likewise, we assume an overlapping sum decomposition of the weighting functions into coarse and fine-scale components denoted by \( \bar{w} \) and \( w' \), respectively.

\[
w(x) = \bar{w}(x) + w'(x) \tag{4.10}
\]

where \( \bar{w}(x) \) and \( w'(x) \) belong to the spaces of functions that accommodate a unique additive decomposition, i.e., \( \mathcal{V} = \bar{\mathcal{V}} \oplus \mathcal{V}' \) and \( \mathcal{V}' = \mathcal{V} \setminus \bar{\mathcal{V}} \). At this point, we make a simplifying assumption on the fine scales that although they are non-zero within the elements, they vanish identically over the element boundaries.

\[
\nu' = w' = 0 \text{ on } \Gamma' \tag{4.11}
\]

**Remark:** Equation (4.11) is not a limitation of the method and it can be relaxed via Lagrange multiplier enforcement of the inter-element continuity of fine-scales.

Expressions (4.7) and (4.10) are substituted in the weak problem (4.5)-(4.6). Assuming that the spaces of coarse- and fine-scales are linearly independent as stipulated in equation (4.8)-(4.9), the two sub-problems become:

**Coarse-scale sub-problem:**

\[
\left( \bar{w}, \frac{\partial (\bar{\nu} + \nu')}{\partial t} \right) - \left( \nabla \bar{w}, (\bar{\nu} + \nu') \otimes (\bar{\nu} + \nu') \right)
+ \left( \nabla' \bar{w}, 2\nu \nabla' (\bar{\nu} + \nu') \right) - (\nabla \cdot \bar{w}, p) - (\bar{w}, f) = 0 \tag{4.12}
\]
\[(q, \nabla \cdot (\overline{\mathbf{v}} + \mathbf{v}')) = 0 \quad (4.13)\]

**Fine-scale sub-problem:**

\[
\left( \mathbf{w}', \frac{\partial (\overline{\mathbf{v}} + \mathbf{v}' \cdot \nabla)}{\partial t} \right) - (\nabla \mathbf{w}', (\overline{\mathbf{v}} + \mathbf{v}') \otimes (\overline{\mathbf{v}} + \mathbf{v}')) \\
+ (\nabla' \mathbf{w}', 2\nu \nabla'(\overline{\mathbf{v}} + \mathbf{v}')) - (\nabla \cdot \mathbf{w}', p) - (\mathbf{w}', f) = 0 \quad (4.14)
\]

The key idea underlying the VMS based turbulence models is to solve the fine scale problem (4.14) locally, and express the fine-scale solution \( \mathbf{v}' \) in terms of the residual of the Euler-Lagrange equations of the coarse scales \( \overline{\mathbf{v}} \). Since \( \mathbf{v}' \) in (4.14) lies in an infinite dimensional space and that the equation is nonlinear, a closed form expression for \( \mathbf{v}' \) is not possible. Consequently, in the discrete case, some approximations need to be made to the space of fine scales \( \mathbf{Y}' \) so as to model \( \mathbf{v}' \). The modeled fine-scale solution can then be variationally projected onto the coarse-scales space, thereby resulting in a modified formulation for (4.12)-(4.13) that only depends on the coarse-scale fields. Furthermore, the contributions of the modeled fine-scales get manifested via the additional residual-based terms that play the role of not only stabilizing the formulation, but also modeling the effects of the sub-grid eddies.

A common procedure adopted for the solution of fine-scale velocity field in the VMS-based turbulence models is the use of Green’s functions based approaches. For general guidelines on the design of Greens’s functions based solutions see Hughes et al. [65], and for an application of the method see Bazilevs et al. [10].

In our work, we treat the fine-scale problem in a rather direct fashion. To find an expression for the fine-scale velocity field we perform linearization of the nonlinear fine-scale problem, and this precludes the need for any a-priori assumption on the form of the fine-scale velocity field. Furthermore, our approach to the fine-scale modeling derives from the notion of the residual free bubbles (RFB) method [17, 39] which is applied only to the fine-scale problem. A form equivalence between the residual-free bubble methods and the Green’s function based methods is presented in Brezzi et al. [16].
4.3.1 Modeling of the fine scale field

We consider the fine scale problem (4.14) and apply integration by parts to the skew term.

\[
(w', \frac{\partial (\bar{v} + v')}{\partial t}) + (w', (\bar{v} + v') \cdot \nabla (\bar{v} + v')) + (\nabla' w', 2v \nabla' (\bar{v} + v')) - (\nabla \cdot w', p) - (w', f) = 0
\]  

(4.15)

where we have employed the assumption on \( w' \) given in (4.11) and have directly enforced the continuity equation (4.6). Rearranging (4.15) we can write:

\[
(w', \frac{\partial v'}{\partial t}) + (w', v' \cdot \nabla v') + (w', \bar{v} \cdot \nabla v')
\]

\[
+ (w', v' \cdot \nabla v') + (\nabla' w', 2v \nabla' v') = - (w', r)
\]  

(4.16)

where

\[
r = \frac{\partial \bar{v}}{\partial t} + \bar{v} \cdot \nabla \bar{v} - 2v \Delta \bar{v} + \nabla p - f
\]  

(4.17)

is the residual of the Euler-Lagrange equations for the coarse scales. Consequently, the projection of the coarse-scale residual onto the fine scales drives the fine-scale problem. Due to the assumption on the space of functions for the fine scales, this residual is defined over the sum of element interiors.

Equation (4.16) presents a time-dependent system of nonlinear equations. To linearize, we use scaling arguments and neglect the higher order term \((w', v' \cdot \nabla v')\). From a computational perspective this amounts to solving the fine scale problem (15) using a single iteration in the Newton-Raphson method for the coarse-scale solution [20]. Assuming the fine-scale velocity to be linear during each of the Newton iterations for the coarse-scales leads to a fine-scale velocity field that scales proportional to the residual, but with a direction that is a linear combination of the directions of the coarse-scale velocity and that of the residual.

We then discretize (4.16) in time using the generalized alpha method [70]. Consequently, at a given time level \( n \), we can write the discrete system as

\[
\left( w', \frac{\partial v'}{\partial t} \right)_{n+\alpha_f} + (w', v'_{n+\alpha_f} \cdot \nabla \bar{v}_{n+\alpha_f}) + (w', \bar{v}_{n+\alpha_f} \cdot \nabla v'_{n+\alpha_f})
\]

\[
+ (w', v'_{n+\alpha_f} \cdot \nabla v'_{n+\alpha_f}) + (\nabla' w', 2v \nabla' v'_{n+\alpha_f}) = - (w', r_{n+\alpha_f})
\]  

(4.18)
where

\[
\frac{\partial v^t}{\partial t}_{n+\alpha_m} = \left( 1 - \frac{\alpha_m}{\gamma} \right) \frac{\partial v^t}{\partial t}_n + \frac{\alpha_m}{\gamma \Delta t} \left( v^t_{n+1} - v^t_n \right) \tag{4.19}
\]

\[
v^t_{n+\alpha_f} = \left( 1 - \alpha_f \right) v^t_n + \alpha_f v^t_{n+1} \tag{4.20}
\]

In equations (4.18) and (4.19), \( \alpha_m, \alpha_f \) and \( \gamma \) are the parameters of the generalized alpha method and \( \Delta t \) denotes the time step increment. Substituting (4.19) and (4.20) in (4.18), and moving the terms at time level \( n \) to the right hand side of the expression, we get

\[
-\left( 1 - \alpha_f \right) \left\{ (w^t, v^t_n \cdot \nabla v^t_n) + (w^t, \bar{v}^t_{n+\alpha_f} \cdot \nabla v^t_{n+1}) + (\nabla^t w^t, 2v^t \nabla^t v^t_{n+1}) \right\}
\]

\[
\frac{\alpha_m}{\gamma \Delta t} \left\{ (w^t, \nabla v^t_{n+\alpha_f}) + (w^t, \bar{v}^t_{n+\alpha_f} \cdot \nabla v^t_n) + (\nabla^t w^t, 2v^t \nabla^t v^t_n) \right\}
\]

\[
= -\left( 1 - \alpha_f \right) \left\{ (w^t, v^t_n \cdot \nabla v^t_n) + (w^t, \bar{v}^t_{n+\alpha_f} \cdot \nabla v^t_n) + (\nabla^t w^t, 2v^t \nabla^t v^t_n) \right\}
\]

\[
-\left( 1 - \frac{\alpha_m}{\gamma} \right) \left\{ (w^t, \frac{\partial v^t}{\partial t}_n) + \frac{\alpha_m}{\gamma \Delta t} (w^t, v^t_n) - (w^t, r^t_{n+\alpha_f}) \right\}
\]

\[
\frac{\alpha_m}{\gamma \Delta t} (w^t, v^t_{n+1} - v^t_n)
\]

\[
\frac{\alpha_m}{\gamma \Delta t} (w^t, v^t_{n+1} - v^t_n)
\]

Remark: We have employed the generalized alpha method in the present work. However, other time integration schemes can also be employed in the modeling of the fine scales by following the general procedure presented here.

4.3.1.1 Evaluating fine-scales via bubble functions approach

In order to solve the discrete problem at time level \( n+1 \), we assume that the fine scales can be expressed in terms of bubble functions, \( b^t(\xi) \), defined over the interior of the elements

\[
v^t = \beta b^t(\xi) \tag{4.22}
\]

\[
w^t = \gamma b^t(\xi) \tag{4.23}
\]

where \( \beta \) and \( \gamma \) are the coefficients for the fine scale velocity trial solutions and weighting functions, respectively. Because of the definition of the bubble functions, the approximation to the localized fine-scale problem is only valid locally, and therefore assumed to be restricted to the element interiors. Consequently, all inner products containing the fine-scale approximations are restricted to element interiors.
Substituting (4.22) and (4.23) in (4.21), we can solve for the fine scale coefficients $\beta_{n+1}$ and construct the fine scale velocity field as

$$v'_{n+1}(x) = b' \beta_{n+1} = \left\{ \frac{\alpha_m}{\gamma \Delta t} (b^e, b^e) + \alpha_f \hat{\tau} \right\}^{-1} \left[ \frac{\alpha_m}{\gamma} (b^e, b^e) - \left( 1 - \alpha_f \right) \hat{\tau} \right] v_n' - \frac{\alpha_m}{\gamma} (b^e, b^e) \frac{\partial v_n'}{\partial t} - b^e (b^e, r_{n+\alpha_f}) $$

(4.24)

where $\hat{\tau}$ is defined as

$$\hat{\tau} = \left[ \int (b^e)^2 \nabla^T \nabla d\Omega + \int b^e \nabla b^e d\Omega I + \nu \int |\nabla b^e|^2 d\Omega I + \nu \int \nabla b^e \otimes \nabla b^e d\Omega \right]^{-1} $$

(4.25)

**Remark:** The tensorial function $\hat{\tau}$ defined in (4.25) is form identical to the tensorial form of the stabilization function derived in Masud and Calderer [97]. Due to the time dependency of the fine-scale velocity in (4.24), the spatial stabilization tensor $\hat{\tau}$ is now fully integrated with the temporal terms that emanate from the ODE integrator.

We can write the fine-scale velocity field in an abstract functional form

$$v'_{n+1}(x) = \mathcal{F} \left( b^e, \hat{\tau}, v_n', \frac{\partial v_n'}{\partial t}, r \right) $$

(4.26)

The expression for the fine-scale velocity field $v'_{n+1}(x)$ is a function of the time history of the fine scales. Furthermore, in the consistently derived fine-scale field given in equation (4.24), the residual $r$ appears inside an integral term. Consequently, a simple definition of the variational operator $\mathcal{T}$ does not emerge that can be easily compared with the traditional so-called stabilization parameters being used in the literature. In the following we will consider various approximation options for the representation of the fine-scale velocity field that are facilitated by the fully coupled space-time system (4.26). Specifically, we will investigate the effects of considering the fine scales to be quasi-static. In other words, we will study the effects of ignoring the time-history of the fine scales. When the time history dependence is ignored, equation (4.24) becomes
This reduction in the temporal domain still yields two options in the spatial dimension:

1. an ability to account for the full spatial variation of the residual, and
2. an option to consider a piecewise constant projection of the residual.

If an element-wise constant projection of the residual $r_{n+\alpha_f}$ is considered, the fine-scale velocity field can be expressed as

$$ v_{n+1}(x) = b^r \beta_{n+1} = -b^r \left\{ \frac{\alpha_m}{\gamma \Delta t} (b^r, b^r) + \alpha_f \hat{\nabla} \right\}^{-1} (b^r, r_{n+\alpha_f}) $$

(4.27)

where

$$ \tau = b^r \left( b^r, 1 \right) \left\{ \frac{\alpha_m}{\gamma \Delta t} (b^r, b^r) + \alpha_f \hat{\nabla} \right\}^{-1} $$

(4.29)

Remark: In the context of incompressible laminar flows [97, 20], to simplify the computation of the fine-scale velocity, we considered the mean value projection of the element-wise residual to be a good approximation, i.e., $(b^r, r_{n+\alpha_f}) \approx (b^r, 1) r_{n+\alpha_f}$. In turbulence modeling, where fine-scales represent the rapidly fluctuating part of the velocity field, it seems
reasonable to consider the full residual. In Sec. 4.4.2.2, we will numerically study the influence of the mean value of the residual versus the full residual on the computed coarse-scale solution.

**Remark:** Fine-scale velocity in equation (4.30) does not depend on its time history. However it retains a term that explicitly depends on \( \Delta t \). In Sec. 4.4.2.5, we will study the effects of ignoring the history dependence of the fine scales on the computed coarse-scale solution.

### 4.3.2 Variational projection of fine-scales onto the coarse-scale space

Now we consider the coarse-scale problem (4.12)-(4.13). Combining the two equations, rearranging terms and integrating by parts the terms that contain spatial derivatives of the fine-scale velocity field \( v' \), the coarse scale problem can be expressed as

\[
B_{\text{Gal}} (\tilde{w}; \tilde{v}) + B_{\text{VMS}}^{\text{Turb}} (\tilde{w}; \tilde{v}, v') = F_{\text{Gal}} (\tilde{w})
\]

(4.31)

where

\[
B_{\text{Gal}} (\tilde{w}; \tilde{v}) = (\tilde{w}, \frac{\partial v}{\partial t}) - (\nabla \tilde{w}, \tilde{v} \otimes \tilde{v}) + (\nabla' \tilde{w}, 2v \nabla' \tilde{v}) - (\nabla \cdot \tilde{w}, p) + (q, \nabla \cdot \tilde{v})
\]

(4.32)

\[
F_{\text{Gal}} (\tilde{w}) = (\tilde{w}, f)
\]

(4.33)

are the standard Galerkin terms, and

\[
B_{\text{VMS}}^{\text{Turb}} (\tilde{w}; \tilde{v}, v') = (\tilde{w}, \frac{\partial v'}{\partial t}) - (\nabla \tilde{w}, v' \otimes v') - (\nabla' \tilde{w}, \nabla' \nabla' \tilde{w} + \nabla q + 2v \Delta \tilde{w}, v')
\]

(4.34)

are the contributions of the fine scales to the coarse-scale problem, which play the dual role of stabilizing the formulation and modeling the effects of the sub-grid scales.

In stabilized methods [62] as well as in the residual-based turbulence methods a \( \text{div} \)-stabilization term is added to the formulation for a more accurate enforcement of the continuity equation or the conservation of mass condition at the element level. This additional term can also be interpreted as the contribution of a fine scale pressure field \( p' \) in the framework of a mixed fine-scale problem. Accordingly, we insert the \( \text{div} \)-stabilization term

\[
b_{\text{div}} (\tilde{w}, \tilde{v}) = (\nabla \cdot \tilde{w}, \tau_e \nabla \cdot \tilde{v})
\]

(4.35)
to the left hand side of (4.31). The parameter $\tau_c$ is defined [10] as

$$
\tau_c = \left(\tau_M \ g \cdot g\right)^{-1}
$$

(4.36)

where $g$ is a second order tensor that is a function of the isoparametric mapping between the spatial and the referential domains. For our model, we define $\tau_M$ to be used in (4.36), as follows

$$
\tau_M = \frac{1}{3} \text{trace}(\tau)
$$

(4.37)

where $\tau$ is the stabilization tensor defined in (4.29) but without the term that contains $\Delta t$. The purpose of using a definition of $\tau_M$ that is independent of $\Delta t$ is to obtain a parameter $\tau_c$ that is well behaved irrespective of the time-step size.

Accordingly, the modified formulation with the $\text{div}$-stabilization term is

$$
B_{\text{Gal}}(\vec{w};\vec{v}) + B^{\text{Turb}}_{\text{VMS}}(\vec{w};\vec{v},\nu') + b_{\text{div}}(\vec{w},\vec{v}) = F_{\text{Gal}}(\vec{w})
$$

(4.38)

**Remark:** The higher order term $(\nabla \vec{w}, \nu' \otimes \nu')$ was neglected in our earlier work on laminar flows [97, 20]. However this term plays a crucial role in the development of residual-based turbulence models presented here.

**Remark:** Motivated by the assumption that the subscales are orthogonal to the coarse scales, some residual-based turbulence models [10, 43] drop the term $(2\nu' \Delta \vec{w}, \nu')$. In Sec. 4.4.2.3 we will investigate the effects of neglecting this term in the formulation on the computed coarse-scale solution.

**Remark:** The $\text{div}$-stabilization term (4.35) when added to (4.31) leads to (4.38). In Sec. 4.4.2.2 the effects of including this additional term to the formulation will be studied.

### 4.3.3 Structure of the fine-scale variational operator

The structure of the fine-scale variational operator that scales the residual of the Euler-Lagrange equations of the coarse scales is given by equation (4.24). In order to understand the structure of this variational operator and to compare it with the classical “stabilization parameters”, it is convenient to consider its reduced form that is attained by considering an
element-wise constant projection of the residual $r_{n+a}$. This amounts to considering the mean value of the residual over element interiors. In addition if we drop the time history terms, it leads to the fine-scale velocity field that is given by equation (4.28). The definition of the stabilization tensor $\tau$ can now be analyzed in this context:

- Tensor $\tau$ has a part which is termed as $\hat{\tau}$ which is defined in equation (4.25). It is composed of the spatial operators of the Navier-Stokes equations acting directly on the fine-scale field. This happens because the standard variational multiscale method belongs to the class of homogeneous multiscale methods wherein the same equation governs the coarse and the fine-scale fields.

- Secondly, and most importantly, equation (4.25) automatically possesses the right order in the advection and the diffusion dominated regimes, i.e., it is $O(1/h)$ and $O(1/h^2)$ in advection and diffusion dominated regions of the solution space, respectively. Attaining the right order in the two flow regimes has been a major design consideration in the development of various stabilization parameters proposed to date [60].

- Another important aspect of the derivation is the dependence of $\tau$ on the temporal domain that is naturally facilitated by the continuous-in-time evolution of the fine-scale velocity field.

- The spatial and temporal terms in the definition of the stabilization tensor are fully coupled with the coefficients of the ODE integrator. This is due to the direct treatment of fine scales via linearization of the fine-scale field and the subsequent full expansion of the time terms in the coupled space-time fine-scale problem.

Lastly, $\tau$ is interpolated via the bubble function and therefore it becomes zero at the element boundaries. In Sec. 4.4.2.1 we will numerically evaluate this $\tau$ and compare it with the state-of-the-art definition of $\tau$ [10] that is commonly used in the VMS community.

**Remark:** An analysis of the spatial component of the stabilization tensor given in equation (4.25) is presented in [97].
4.4 Numerical results

The validity and accuracy of the proposed formulation is shown by means of three test problems. The first problem is forced-isotropic turbulent flow, where energy is supplied at a constant rate to the lower velocity modes. This test case is used to check if in the inertial subrange, the proposed method is transferring energy to shorter wavelengths at the theoretically predicted rate. The second test case is a turbulent channel flow. We use this problem to study the effects of various modeling options, discussed in Sec. 4.3, on the physics of the wall-bounded flows. Finally, the third problem investigates the flow around a fixed cylinder at $Re = 3,900$. This problem is more complex than the former two because it contains two boundary layers that detach from the cylinder in a statistically periodic fashion.

All through our numerical calculations we have employed the formulation given in equation (4.38) as our baseline method. This formulation accounts for the second derivative term $(2\nu \Delta \mathbf{w}, \nu')$ and the fine scale pressure field, i.e., the div-stabilization term. In addition, the baseline formulation employed in the numerical studies uses the fine scale velocity obtained in (4.28) that omits the time-history of the fine scales, along with the element-wise mean value of the residual $\mathbf{r}$. For test cases where the baseline formulation is not used, we clearly state the changes.

In all the test cases, 8-node hexahedral elements are used, and full numerical quadrature is employed for spatial integration [61]. Standard quadratic bubble function is employed to solve the fine-scale problem. It is important to note that if the same bubble function is employed everywhere in the evaluation of the $\hat{\nu}$ presented in (4.25), then the skew-symmetric term would vanish for the case of a uniform velocity field. In [96] we proposed a method based on the idea of residual-free bubbles to modify the bubble function that is employed in the weighting slot of the skew-advection term. In the residual-free bubbles method, a residual-driven problem is solved at the element level [17]. In general, it is not possible to find the exact residual-free bubbles unless the exact solution to the problem is known. Therefore, a method was proposed by Brezzi et al. [17] to approximate the residual free bubbles using pyramidal bubbles wherein the location of the center of the pyramid is evaluated via minimizing the $L_2$-norm of the residual. Motivated by [17] we define the bubble function that appears in the weighting slot of the advection term in (4.25) to be the shape
function associated with the most up-winding node of the element. For a detailed description of the procedure for choosing the modified bubble function, see [97].

The time discretization scheme employed is the generalized alpha method, with parameter $\rho_{\infty} = 0$. For preconditioning, the default Additive-Schwartz Method (ASM) preconditioner provided in PETSc is used that employs injection restriction and the transpose for interpolation. In addition, the stabilized bi-conjugate method is used to solve the linear systems that arise from the linearization of the nonlinear equations.

### 4.4.1 Forced isotropic turbulence

We first consider the forced isotropic turbulence problem. The problem characteristics and the driving mechanism are the same as the ones presented in [10]. Constant power is supplied to the lowest velocity modes of the fluid via external forcing function which is defined as

$$f(x) = \sum_{k,|k| \leq k_f} \frac{P_{in}}{2E_{k_f}} \hat{u}_k e^{i{k} \cdot x}$$

where $i$ is the imaginary unit, $P_{in} = 62.8436$ is the constant power input to the flow,

$$E_{k_f} = \frac{1}{2} \sum_{k,|k| \leq k_f} \hat{u}_k \cdot \hat{u}_k$$

is the contribution of the lowest velocity modes to the kinetic energy, and

$$\hat{u}_k = \frac{1}{|k^2|} \int_{\Omega} u(x) e^{-i{k} \cdot x} d\Omega$$

are the Fourier coefficients of velocity associated with wave-number $k$. The parameter $k_f$, which is the threshold that defines the limit of the lowest modes, is set equal to 2.

The computational domain is a cube of length $2\pi$ with periodic boundary conditions applied at the six faces. Kinematic viscosity $\nu$ is set equal to $1/150$, and therefore, the Taylor micro-scale Reynolds number $Re_\lambda$ is 165. The domain is discretized with uniform meshes of $32^3$ and $64^3$ hexahedral elements. Time step $\Delta t$ is set equal to $5 \times 10^{-3}$ and $2.5 \times 10^{-3}$ for the two meshes, respectively.
The problem is allowed to evolve in time until a dynamically equilibrated state is reached. Once in the dynamically equilibrated region, the problem is run for additional time steps, and following the guidelines given in [10], statistical data is collected. We observed that 10 units of time are enough to reach the statistically equilibrated state. The average kinetic energy density $q$ of the problem is obtained as

$$q^2 = \frac{1}{2|\Omega|} \int_{\Omega} \mathbf{u}(x) \cdot \mathbf{u}(x) \, d\Omega$$

(4.42)

In all the three meshes, $q$ is about $41.5 \pm 20\%$ which agrees with the values reported in [10]. Figure 4.1(a) shows velocity streamlines and vorticity iso-surfaces at a given time level obtained with $64^3$ mesh. Details of the vorticity structures surrounded by velocity streamlines can be observed in Figs. 4.1(b,c). Figure 4.2 shows the Fourier transform of the auto-correlation function, which confirms that the rate at which energy is transferred to the higher wave-numbers coincides with the theoretically predicted rate.

The two-point third-order correlation function, which is represented in Fig. 4.3, is defined as

$$S_3(r) = \left\langle (u_i(x + r e_i) - u_i(x))^3 \right\rangle$$

(4.43)

where $u_i$ and $e_i$ are the $i$-th components of the velocity and the unit vector in the $i$-th direction, respectively. As can be seen in Fig. 4.3, our solution converges to the DNS solution as the mesh is refined.

### 4.4.2 Turbulent channel flow

Turbulent channel flow is a standard benchmark problem for evaluating the accuracy of turbulence models in wall bounded flows. In this section channel flow is studied for two different Reynolds numbers, $Re_T = 395$ and $Re_T = 590$. Results are compared with DNS results of Moser and co-workers [103], with VMS results [10, 43] and with LES results obtained with a dynamic Smagorinsky model [43]. Furthermore, in the context of the turbulent channel flow we study the behavior of our fine scales models and investigate the various modeling options that were discussed in Sec. 4.3. The modeling assumptions that we use in the following sections are summarized in Table 4.1.
We consider a hexahedral channel with dimensions \( L_x \times L_y \times L_z \). No-slip boundary conditions are prescribed at the walls that are normal to the \( y \)-direction. Periodic boundary conditions are prescribed along the other two directions. A constant body force, \( f \), is applied to the fluid along the \( x \)-direction. Figure 4.4 shows a schematic representation of the channel. We consider a flow where \( f_x = 0.00337204 \) and \( \nu = 0.0001472 \). Based on the wall units [113], Reynolds number \( Re_T = 395 \). For the second flow that we study, we set \( f = 1.0 \) and \( \nu = 0.001694915 \), which leads to \( Re_T = 590 \). For \( Re_T = 395 \) flow, the dimensions of the channel are \( 2\pi \times 2 \times (2/3)\pi \), and for the \( Re_T = 590 \) flow, channel dimensions are \( 2\pi \times 2 \times \pi \).

The domain is discretized with meshes of \( 32^3 \) and \( 64^3 \) hexahedral elements. The elements are uniformly distributed in the \( x \) and \( z \)-directions, while in the wall-normal direction, elements are graded using a hyperbolic stretching. With the exception of Sec. 4.4.2.5, where a time step study is carried out, we set time step \( \Delta t = 0.025 \) for \( Re_T = 395 \) flow, and \( \Delta t = 0.0015 \) for \( Re_T = 590 \) flow.

The simulations are initialized with a perturbed Poiseuille flow. For each of the cases presented below, the problem is run until a statistically steady state regime is reached. Once the flow is in the statistically steady state regime, the simulation is continued and the solution is sampled every 10 time steps.

### 4.4.2.1 Numerical study of the stabilization tensor

In Sec. 4.3 the fine-scale field is modeled using a bubble-functions approach, while other residual-based turbulence models compute the fine-scale velocity field using Green’s functions along with heuristic simplifications [10]. Here we compare our derived stabilization tensor \( \tau \) obtained from (4.28) with the one used in [10], which is expressed as

\[
\tau = \tau_M I \tag{4.44}
\]

The parameter \( \tau_M \) is defined as

\[
\tau_M = \left( \frac{4}{\Delta t^2} + \vec{F} \cdot \vec{G} + C_f \nu^2 \vec{G} : \vec{G} \right)^{-1/2} \tag{4.45}
\]

where the second order tensor \( \vec{G} \) is defined as
in which \( x = x(\xi) \) is the mapping between the coordinates \( \xi = \{ \xi_i \}_{i=1}^3 \) expressed in the isoparametric space of the element and the coordinates \( x = \{ x_i \}_{i=1}^3 \) expressed in the physical space.

For the turbulent channel flow at \( Re_T = 395 \), Fig. 4.5(a) shows the stabilization parameter plotted along a line orthogonal to the wall that has prescribed no-slip boundary condition. This line passes through the centerline of a column of elements. Since the stabilization parameter in (4.28) is pre-multiplied by the bubble function, it attains a value \( \tau = 0 \) along element boundaries. Accordingly, the intercept along horizontal axis in Fig. 4.5(a) represents the inter-element boundaries. The mesh employed for turbulent channel flow is graded in the wall normal direction, and therefore we see the graded spatial support for the bubbles. We also observe a reduction in \( \tau_{\max}(\Omega') \) close to the bounding wall. Since our stabilization parameter is in fact a tensor quantity, we use one third of the trace of the tensor for comparison purposes. Also plotted is the classical \( \tau_M \) [10] defined in (4.45). For comparison, in Fig. 4.5(b) we plot the element-wise mean value of the parameter

\[
\tau_{AVG} = \frac{1}{\Omega^e} \frac{1}{3} \text{trace}(\tau) d\Omega
\]  

(4.47)

in the wall normal direction. The figure shows that the value of \( \tau_{AVG} \) over the element is in the same range as the value of \( \tau_M \) from (4.45) and therefore our derived stabilization tensor behaves analogous to the classical stabilization parameter [60, 10]. In our numerical implementation, we have employed the full \( \tau \) that varies over the element because of composition with the bubble function.

### 4.4.2.2 Study of the effects of accounting for the fine-scale pressure field

Equation (4.31) is the result of considering a multiscale decomposition of the velocity field alone, i.e., a decomposition of the pressure field into coarse- and fine-scale pressures is not considered. Some residual-based turbulence models assume the existence of a fine-scale
pressure field \[10\], that manifests itself as an additional term that is proportional to the divergence of the coarse-scale velocity field. Consequently, it results in a more accurate enforcement of conservation of mass in an element wise fashion. In order to have a better enforcement of the continuity equation, we have added a div-stabilization term in (4.31), which yields a modified formulation (4.38). The purpose of the present section is to study the influence of this additional term, and therefore of the assumption of the existence of a fine-scale pressure field on the computed large-scale features of the VMS-based turbulence model. For the simulations presented in this section, we have employed an element-wise constant projection of the coarse-scale residual given in equation (4.28) that ignores the time-history of the fine scales.

For the turbulent flow at \(Re_T = 395\) and for the \(32^3\) elements mesh, Fig. 4.6 shows snapshots of the streamlines and vorticity iso-surfaces at various time levels. Also presented is the velocity field projected onto the walls of the channel. The convection of mass-less particles in the boundary layer region is shown and the particles are color coded to indicate their age as the simulation progresses. The boundary layer region is clearly evident and the effect of turbulent fluctuations can be observed via the randomness in the motion of the particles as they age.

Figure 4.7 shows the mean-stream velocity and the root mean square (R.M.S.) of the fluctuations of the velocity field for the \(32^3\) elements mesh. Both of our formulations (4.31) and (4.38) are considered. The results are compared with the DNS results of Moser et al. [103]. For comparison purposes, Fig. 4.7 also includes results obtained with a Smagorinsky model [43] and VMS results reported by Bazilevs and co-workers [10] using a mesh of tri-linear hexahedral \(32^3\) elements, where a fine scale pressure field was included. Figure 4.7 also shows the results presented in [10] using an equivalent mesh but with cubic NURBS. We see that our results with \(p'\) are similar to the results reported in [10] for linear elements. It can also be observed that the mean-stream velocity and the fluctuations in the stream-wise and wall-normal directions are better captured with the formulation that does not consider the fine-scale pressure field (4.31). However, Table 4.2 shows that not accounting for the fine-scale pressure results in a poorer enforcement of the element-wise continuity equation. Fluctuations of the velocity in the span-wise direction are represented equally well with both the formulations (4.31) and (4.38).
Figure 4.8 shows a study carried out using a $64^3$ elements mesh and comparison is done with the results obtained with the cruder mesh of $32^3$ elements. Figure 4.9 shows results for the turbulent channel flow at a higher Reynolds number $Re_T = 590$ for the $64^3$ hexahedral elements mesh. As can be seen, formulation (4.38) performs better than the results obtained with a VMS model presented in [43] where $64^3$ hexahedral elements mesh was also used.

**Remark:** It is well documented in the literature that lower order Lagrange elements have a propensity for volumetric locking when the incompressibility condition given in equation (4.2) is strongly enforced [61, Chapter 4]. On one hand the fine-scale pressures that manifest themselves in the form of an additional div-stabilization term help in the enforcement of the continuity equation, on the other hand they tend to make the response rather overly stiff. We see these effects in Figure 4.7 where ignoring the div-stabilization term results in a flexible response that is better able to represent the mean flow statistics as well as the fluctuations. However, considering the relative importance of satisfying the continuity equation, we consider formulation (4.38) that accounts for $p'$ as our base formulation hereon.

As discussed in Sec. 4.3, adding a fine-scale pressure field is a way to strengthen the continuity constraint. Table 4.2 shows the time averaged $L_2$-norm of the divergence of the velocity field, $\left\langle \| \nabla \cdot \bar{v} \|_{L_2} \right\rangle$. It can be seen that, although the mean velocity field and its fluctuations are invariably better captured with the formulation that does not account for the fine-scale pressure field $p'$, the incompressibility constraint is better satisfied if the fine-scale pressure is taken into account. Satisfaction of the incompressibility constrain is an important consideration in the solution of the incompressible Navier-Stokes equations, as it is directly related to the satisfaction of the local conservation of mass. As presented in Table 4.2, an increase in $Re_T$ results in a reduction in the accuracy of the local conservation property. Consequently, accounting for this term, especially for higher $Re_T$ flows would seem necessary.
4.4.2.3 Study of the effect of employing the mean-value of the residual

In Sec. 4.3.2, where the fine-scale problem is modeled, the representation of the fine-scale velocity field can be simplified by assuming an element-wise constant projection of the residual of the coarse-scale equations. If the full residual is taken into account, then fine-scale solution is exactly a quadratic bubble function. However, if the mean-value projection is considered, then the fine-scale solution is a modulated quadratic bubble function. In this section we study the effects of the reduced order projection of the element-wise residual on the statistics of the numerical solution for the turbulent channel flow at $Re_T = 395$. Specifically, we use the mean-value based fine-scale field given in (4.28), and compare it with the case wherein the full residual is employed only in the higher-order terms in (4.27) while in the rest of the terms we still consider the mean-value based residual. We employ our standard formulation (4.38) that takes into account the fine-scale pressure term, and also ignore the time-history of the fine-scales in the evaluation of the fine scales. Figure 4.10 shows the statistics for the two cases. In both cases, the $32^3$ elements mesh is employed. It can be seen that there is no appreciable improvement in the solution even if the full residual is used.

4.4.2.4 Study of the effects of the orthogonality of sub-scales

To study the effects of the orthogonality of sub-scales with respect to the coarse scale space, we investigate the flow at $Re_T = 395$. We employ our standard formulation (4.38) that accounts for the term $(2\nu \Delta' \vec{w}, \nu')$, and compare it with the case wherein fine-scales are orthogonal to the coarse-scales, thereby, annihilating $(2\nu \Delta' \vec{w}, \nu')$. For this study we have employed an element-wise constant projection of the coarse-scale residual given in equation (4.28) wherein history dependence of fine-scales is suppressed. The study was performed using the $32^3$ elements mesh. Figure 4.11 shows the statistics for the two formulations, where the two results are practically coincident.

Remark: With a view that the fine scale viscosity term $(2\nu \Delta' \vec{w}, \nu')$ might be introducing excessive fine scale dissipation, the notion of the orthogonality of sub-scales with respect to the coarse scale space has been employed in the literature as a means to annihilate this term.
4.4.2.5 Study of the effects of neglecting the time-history of fine-scales

As discussed in Sec. 4.3, equation (4.26) offers several options for the time-dependency of the fine scale velocity field. Specifically, two models for the velocity fine scales are considered. In the reduced model, given in (4.28), the time history of the fine-scales is neglected, however the variational operator \( \tau \) still retains the dependence on \( \Delta t \). In the full model, given in (4.24), the fine scales are time-dependent and they need to be tracked at Gauss points if an element-wise constant projection of the residual is to be considered. The version of the full model presented in this section assumes an element-wise constant projection of the residual (4.30).

To compare the two models we analyze the turbulent channel flow at \( Re_T = 395 \) and perform a time step study with \( \Delta t = 0.025 \) and 0.00625. For the case of dynamic fine-scales, time step \( \Delta t = 0.0015625 \) is also employed. In both the cases, the \( 32^3 \) elements mesh is employed. Figure 4.12 shows the results obtained with the first model that omits the history dependence of the fine scales. It can be seen that as \( \Delta t \) is decreased, the results do not converge. The degradation in accuracy as \( \Delta t \) is decreased is clearly manifested via the fluctuations in the wall-normal and span-wise velocities in Figs. 4.12(c) and 4.12(d), respectively. This anomaly can be explained by observing equation (4.28), where in the limit \( \Delta t \to 0 \) the fine scales vanish, and as a consequence, the stabilization terms in the formulation also vanish. On the other hand, Fig. 4.13 shows that for the model that accounts for the history dependence of fine-scale field, very small time steps do not degrade the accuracy of the solution. Similar behavior for analogous models has also been reported in Hsu et al. [55] and Gamnitzer et al. [43].

It is important to note that the computation of quasi-static fine scales is computational economical as compared to the dynamical fine scales. Therefore, when the step-size is large, dropping the time history of the fine scales leads to computational economy. On the other hand, the quasi-static fine scales show a pathological behavior when a very small time step size is employed. Consequently, when very small time steps are required, the model that takes into account the history of the fine-scales should be used as it produces more accurate results.
4.4.3 Turbulent flow around a fix cylinder

Viscous flow around a circular cylinder at sufficiently high Reynolds number is a classical benchmark problem that leads to periodic vortex shedding commonly known as the Karman vortex street. In this section we study the flow around a circular cylinder in the turbulent regime and compare our results with the LES results reported in Kravchenko and Moin [79]. In [79], a numerical method based on B-splines was employed. We also compare our results with experimental data reported in Ong and Wallace [111] and with experiments reported in [79] that were conducted by Norberg, and Lourenco and Shish.

We consider a unit diameter cylinder that is centered in the domain as schematically presented in Fig. 4.14. Viscosity is set equal to $2.5641 \times 10^{-4}$. The Reynolds number based on the inflow velocity and diameter of the cylinder is 3,900. No-slip boundary condition is imposed on the surface of the cylinder. Velocity on the inflow boundary is set equal to 1, periodic boundary conditions are imposed in the $z$-direction, while no-penetration and zero tangential stress conditions are prescribed on the lateral walls. Zero stress is prescribed on the outflow boundary.

Following the guidelines given in [79], the domain is discretized in 48 layers of elements. Each layer approximately contains 160 elements in the radial direction and 250 elements in the circumferential direction. This gives rise to a mesh that consists of 2,436,819 nodes and 2,370,144 hexahedral elements. The mesh is uniform in the direction of the axis of the cylinder and graded in the other directions so that the region with the highest density of elements lies downstream from the cylinder. Details of the mesh around the cylinder can be seen in Fig. 4.15. Time step $\Delta t$ is set equal to 0.0025.

The grid employed in [79] has 1,333,472 points. In its local resolution it is comparable to the meshes considered in this section in the vicinity of the cylinder and in its wake. However, the present meshes have more elements in the rest of the domain. A better mesh generator would have yielded an optimal mesh with lesser grid points than are there in our meshes.

In this section we have employed the formulation that includes the fine-scale pressure field. However, we have opted to ignore the time history of the fine scale velocity field.
 Starting from a zero initial velocity, the problem is allowed to evolve until the main features of the flow are fully developed. Figure 4.16 shows that the flow consists of two laminar boundary layers that detach from the cylinder and transition into turbulent layers downstream from it. Figures 4.16(a,b) show vorticity iso-surfaces at two instants of time that are approximately half cycle apart. During the post processing of the data, mass-less particles were injected in a plane located upstream of the cylinder. The sequence of images 4.16(a,b) show that, as time progresses, the particles are convected by the fluid and they reveal the turbulent regime of the flow downstream from the cylinder. The color of the particles indicates their age, with the darkest particles being the oldest. Likewise, images 16(c,d) show zoomed view of velocity streamlines and vorticity iso-surfaces where velocity magnitude is employed to color the streamlines, and pressure is employed to color the iso-surfaces.

Once the flow is fully developed, it is sampled every 20 time steps for the next 30 units of time. The statistics of the velocity and pressure fields of the fluid are computed by averaging the solution fields over time and over space along the direction of the axis of the cylinder; a direction in which the flow is homogeneous. Figure 4.17 shows the mean pressure field on the surface of the cylinder. The results are comparable with the B-spline results and Norberg’s results [79]. Figure 4.17 also shows the results obtained with the present formulation but with a mesh that consists of 1,854,720 nodes and is much coarser in the boundary layer region compared to our base mesh. A good agreement with [79] can also be observed in Fig. 4.18, where the mean velocity is plotted along the x-direction. Figure 4.18 also contains the result obtained with our coarser mesh. Figure 4.19 shows the mean stream-wise velocity along three different transverse sections located at $x=1.06$, $x=1.54$ and $x=2.02$ with respect to the center of the cylinder. Analogously, Fig. 4.20 shows the mean transverse velocity along the same three transverse sections. Figure 4.21 plots the mean stream-wise velocity along the sections $x=6.0$, $x=7.0$ and $x=10.0$ with respect to the center of the cylinder. In all the cases a good agreement with previously published results [79] is attained. Additionally, Figs 4.19 and 4.21 show good agreement with experimental results.

Figure 4.22 shows the stream-wise velocity fluctuations along three transverse sections. Similarly, Fig. 4.23 shows the Reynolds shear stress along these transverse sections. In both the cases, the present results are in good agreement with the published results [79, 111].
4.5 Conclusions

We have presented a residual-based Large Eddy Simulation model for incompressible turbulent flows. The proposed model differs from other VMS-based turbulence models in that a residual-free bubbles approach has been adopted to derive an analytical expression for the structure of the fine-scale variational operator $\mathbf{\tau}$. A direct treatment of the fine scale problem with bubble functions precludes the need for any modeling assumption on the form of the fine scales, and this constitutes the turbulence modeling paradigm within the VMS framework.

The proposed model has been implemented for the 8-node hexahedral elements, and numerically validated using three test cases of increasing degree of complexity: forced isotropic turbulence flow, turbulent channel flows at various Reynolds numbers, and turbulent flow around a cylinder. In all the cases, we have shown that our results compare very well with the results obtained via the traditional LES models, as well as with other VMS-based turbulence models.

The application of the bubble functions approach to the solution of the fine-scale problem offers several simplifying approximations for the representation of the fine scale fields. Employing the turbulent channel flow as a test case, we have investigated the effects of these modeling options. In particular, we have shown that an additive decomposition of the pressure field into coarse and fine scales provides a tighter control on the enforcement of the incompressibility constraint. On the other hand, if the fine-scale pressure is ignored, a general improvement in the mean flow statistics as well as in the fluctuations of the velocity components is observed. This improvement however comes at the cost of a loss in the local conservation property as the Reynolds number is increased. For the test cases employed here, the assumption of orthogonality of the fine-scales did not seem to affect the computed coarse scales in any appreciable way. Furthermore, we showed that instead of projecting the full coarse-scale residual onto the fine-scale space to drive the fine-scale problem, employing an element-wise mean-value projection of the residual provides good accuracy in the computed coarse scales. Finally, we also confirm the phenomenon observed in [55, 43] that if the dynamic effects of the fine-scale velocity are neglected, the stabilization feature of the formulation diminishes for very small time step sizes. However, if the fine-scales are
considered to be time-dependent, the resolved coarse-scale features of the model stay uniformly stable and accurate even for very small time step sizes.

4.6 Figures and tables

![Vorticity iso-surfaces and velocity streamlines, 64³ elements mesh. (a) Full view of the problem domain, (b, c) two different close-up views. This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.](image)
Figure 4.2 Fourier transform of the 1D autocorrelation function

Figure 4.3 Two-point third order correlation function

Figure 4.4 Schematic representation of the channel
Figure 4.5 Comparison of stabilization parameter. (a) Actual computed value (b) Averaged value over the element
Figures 4.6 (a-c) Streamlines, vorticity iso-surfaces, velocity field projected onto the walls, and massless particles in the boundary layer region for the turbulent channel flow at $Re_T = 395$. (32$^3$ elements mesh). This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.
Figure 4.7 Effects of accounting for the fine-scale pressure field. $Re_T = 395$, 32$^3$ elements mesh. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 4.8 Effects of mesh refinement on the computed solution. $Re_T = 395$, $32^3$ and $64^3$ elements mesh. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 4.9 Effects of accounting for a fine-scale pressure field. $Re_T = 590$, $64^3$ elements mesh. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions
Figure 4.10 Effects of considering a constant-projection of the residual. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 4.11 Effects of considering orthogonal sub-scales. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 4.12 Study of $\Delta t$ refinement when dynamic effects of fine-scales are partly neglected. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 4.13 Study of $\Delta t$ refinement when all dynamic effects of fine-scales are considered. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions
thickness of the domain: $\pi$

**Figure 4.14** Schematic representation of the cylinder problem

**Figure 4.15** Plan zoomed view of the upper half of the mesh around the cylinder
Figure 4.16 (a,b) Vorticity iso-surfaces colored with the velocity field at two different time instants, and (c,d) zoomed view of velocity streamlines and vorticity iso-surfaces where velocity magnitude is employed to color the streamlines and pressure is employed to color the iso-surfaces. This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.
Figure 4.17 Mean pressure on the surface of the cylinder. The stagnation point corresponds to $\theta = 0$.

Figure 4.18 Mean velocity along the stream-wise direction $y = 0$. 
Figure 4.19 Mean stream-wise velocity along (a) $x = 1.06$, (b) $x = 1.54$, and (c) $x = 2.02$
Figure 4.20 Mean transversal velocity along (a) $x = 1.06$, (b) $x = 1.54$ and (c) $x = 2.02$
Figure 4.21 Mean stream-wise velocity along (a) $x = 6.00$, (b) $x = 7.00$
and (c) $x = 10.0$
Figure 4.22 Mean stream-wise velocity fluctuations along (a) $x = 6.00$, (b) $x = 7.00$ and (c) $x = 10.0$
Figure 4.23 Mean Reynolds shear stress along (a) $x = 6.00$, (b) $x = 7.00$ and (c) $x = 10.0$
Table 4.1 Summary of numerical models employed in each of the sub-sections of the turbulent channel flow problem

<table>
<thead>
<tr>
<th>Section</th>
<th>Purpose of the section</th>
<th>Observations</th>
<th>Fine-scales</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4.2.1</td>
<td>Compare behavior of $\tau$ defined in equation (4.29) with $\tau$ defined in [10].</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>4.4.2.2</td>
<td>Study the effect of $p'$.</td>
<td>Fine-scales are quasi-static, non-orthogonal and mean residual is considered.</td>
<td>(4.28)</td>
</tr>
<tr>
<td>4.4.2.3</td>
<td>Study the effect of the mean-value of the residual vs. the full variation of it.</td>
<td>Fine-scales are quasi-static and non-orthogonal.</td>
<td>(4.27) and (4.28)</td>
</tr>
<tr>
<td>4.4.2.4</td>
<td>Study the effect of using orthogonal fine-scales vs. non-orthogonal fine-scales.</td>
<td>Fine-scales are quasi-static, and mean residual is employed. $p'$ is included.</td>
<td>(4.28)</td>
</tr>
<tr>
<td>4.4.2.5</td>
<td>Study the effect of considering transient fine-scales vs. quasi-static fine-scales.</td>
<td>Fine-scales are non-orthogonal and mean residual is employed. $p'$ is included.</td>
<td>(4.28) and (4.30)</td>
</tr>
</tbody>
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Table 4.2 Time-averaged $L_2$-norm of the divergence of the velocity $\left\langle \left\| \nabla \cdot \mathbf{v} \right\|_2 \right\rangle / \left\| \mathbf{v} \right\|_2$

<table>
<thead>
<tr>
<th>$Re_T$</th>
<th>$p' = 0$</th>
<th>$p'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re_T = 395$ (32³ elements mesh)</td>
<td>$1.49 \times 10^{-1}$</td>
<td>$1.93 \times 10^{-2}$</td>
</tr>
<tr>
<td>$Re_T = 590$ (64³ elements mesh)</td>
<td>$6.32 \times 10^2$</td>
<td>$1.67 \times 10^1$</td>
</tr>
</tbody>
</table>
Chapter 5

Residual-based Variational Multiscale turbulence models
for unstructured tetrahedral meshes

5.1 Motivation

Large Eddy Simulation (LES) is a numerical technique that resolves the larger features in the flow and models the effects of the smallest features. It is a powerful tool to study turbulent flows [118, 81, 44, 29, 68, 102, 85] and is computationally less expensive than Direct Numerical Simulations [103] that try to resolve for all the scales in the problem.

This Chapter presents a residual-based turbulence model that is derived via a nested application of the Variational Multiscale (VMS) ideas. The VMS framework assumes an overlapping additive multiscale decomposition of the continuous fields into coarse and fine-scale components and it was proposed by Hughes [64] as the basis for stabilized methods. Variational Multiscale ideas were extended to develop turbulence models [65, 66, 67, 26, 106] where coarse- and fine-scales were interpreted as the low and high wave numbers that were associated with large and small physical features in the flow. Some recent works that employ VMS ideas are [78, 47, 35, 10, 25, 2, 11, 43, 55] wherein larger structures in the flow are numerically resolved and finer structures are modeled, a feature that is common with the LES modeling ideas.

The present Chapter is an extension of Chapter 4, in which the development of residual-based turbulence models for the incompressible Navier-Stokes equations was presented. In Chapter 4, we assumed an overlapping additive split of only the velocity field, while the pressure field was not segregated into coarse and fine-scale components. Consequently, the fine-scale problem was a function of the coarse and fine velocity and coarse pressure field. A bubble functions based approach was adopted to extract a model for the spatio-temporal fine-scale velocity field that was embedded in the coarse-scale problem to yield the residual-based turbulence model. Numerical investigations with the method prompted us to add an element level divergence term for an improved representation of the
local mass conservation property. This formulation worked well for linear hexahedral 
elements and a variety of benchmark tests were done. An application, of the method to 
tetrahedral element meshes yielded numerical results that manifested the inherent stiff 
response of lower order tetrahedral elements that has also been reported in the literature [114]. 
This prompted us to revisit our line of thought for the residual-based turbulence models [98] 
that was based on a less restrictive representation of fine-scale velocity by making it time 
dependent, as compared to our earlier works on convection dominated flows [89, 92, 97, 20] 
where fine velocity was assumed piece-wise constant in time. In other words, a less restrictive 
representation of fine velocity resulted in a refined model for fine scales and therefore yielded 
a residual-based turbulence model. Our motivation in this work is to extend this line of 
thought to develop a refined representation of the fine-scale velocity and pressure fields that 
could compensate for the inherent stiff response of the low-order tetrahedral elements.

This Chapter presents refined models for the fine-scale velocity and pressure fields 
that are derived via a nested and hierarchical application of the VMS method. From the onset, 
we assume a multiscale decomposition of both the velocity and pressure fields. Consequently, 
the problem that governs fine scales is also a mixed field problem, and therefore it needs to be 
stabilized if arbitrary interpolation functions are to be used for fine-scale velocity and pressure. 
To accomplish this, we perform another application of the VMS ideas, and further decompose 
the fine-scale velocity in two overlapping components termed as fine-scales level-I and level-
II. The goal of level-II scales is to provide VMS based stabilization to the problem governing 
level-I scales. A subsequent variational projection of the fine-scales obtained from the 
stabilized level-I problem to the coarse-scale problem yields the turbulence model. While the 
coarse scales are interpolated using standard shape functions, level-I and level-II scales are 
modeled employing bubble functions. The presence of fine-scale pressure field allows us to 
consistently derive terms that are analogous to the “\textit{div}-stabilization” term, and they help 
improve the conservation of mass property in the model. We delineate on this aspect further 
in Sec. 5.3.1.

The remaining part of the Chapter is organized as follows. The Navier-Stokes 
equations and their weak formulation are presented in Sec. 5.2. In Sec. 5.3 we derive the 
three-scale residual-based turbulence model employing the variational multiscale framework. 
In Sec. 5.3 the development of the fine-scale models is presented in detail and the various
modeling assumptions taken into consideration are discussed. In Sec. 5.4 several numerical tests are presented to show the accuracy of the formulation for unstructured tetrahedral meshes. In Sec. 5.4.1 we consider a turbulent channel flow which is a classical benchmark problem for turbulence models. We compare our results with reference DNS solutions and with other LES models published in the literature [10, 98]. We also propose some modeling simplifications for computational economic considerations and study the effect of some of these simplifications, namely, the effect of the diagonalization of the second order tensor $\boldsymbol{\tau}$ that arises in the derivation of the turbulence models. The effects of the modeling simplifications that affect the temporal domain are also investigated. In Sec. 5.4.2 we study flow around an airfoil at Reynolds numbers 60,000 to show the applicability of our method to more complex problems. Conclusions are drawn in Sec 5.5.

5.2 The incompressible Navier-Stokes equations

Let $\Omega \subset \mathbb{R}^3$ be a connected, open, bounded domain with piecewise smooth boundary $\Gamma$. Let $\mathbf{v} : \Omega \times ]0, T[ \rightarrow \mathbb{R}^3$ be the velocity field and $p : \Omega \times ]0, T[ \rightarrow \mathbb{R}$ the kinematic pressure field. The incompressible Navier-Stokes equations consist of solving the following set of equations on the space-time domain $\Omega \times ]0, T[$, where $T > 0$:

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v} \otimes \mathbf{v}) - 2\nu \nabla \cdot \varepsilon(\mathbf{v}) + \nabla p = \mathbf{f} \quad \text{in } \Omega \quad (5.1)$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega \quad (5.2)$$

$$\mathbf{v} = g \quad \text{on } \Gamma \quad (5.3)$$

$$\mathbf{v}(x,0) = \mathbf{v}_0 \quad \text{in } \Omega \quad (5.4)$$

where $\mathbf{f} : \Omega \times ]0, T[ \rightarrow \mathbb{R}^3$ is the body force (per unit of mass), $\nu > 0$ is the kinematic viscosity (assumed constant), $\mathbf{v}_0$ is the initial condition for the velocity field which satisfies the condition that $\nabla \cdot \mathbf{v}_0 = 0$, $g$ represents the Dirichlet boundary conditions, and $\otimes$ denotes the tensor product. The second order tensor $\varepsilon(\mathbf{v})$ is the strain-rate tensor which is defined as $\varepsilon(\mathbf{v}) = \nabla \mathbf{v} = \left[ \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right]/2$. Equation (5.1) is the momentum balance equation; equation
(5.2) is the incompressibility constraint; equations (5.3) is the Dirichlet boundary condition; and (5.4) is the initial condition.

Let $w(x) \in V = \left( H^1_0(\Omega) \right)^3$ and $q(x) \in Q = C^0(\Omega) \cap L^2(\Omega)$ represent the weighting functions for the velocity and pressure fields, respectively. The appropriate spaces of functions for the velocity and pressure trial solutions are the corresponding time-dependent spaces $S$ and $P$ that satisfy the initial and boundary conditions. The standard weak form of the problem defined in (5.1)-(5.4) is: Find $v(x,t) \in S$ and $p(x,t) \in P$ such that for all $w(x) \in V$ and $q(x) \in Q$,

\[
(w, \frac{\partial w}{\partial t}) - (\nabla w, \nu \otimes v) + (\nabla' \nu, 2\nu \nabla' v) - (\nabla \cdot w, p) = (w, f) \quad (5.5)
\]

\[
(q, \nabla \cdot v) = 0 \quad (5.6)
\]

where $(\cdot, \cdot) = \int_{\Omega} (\cdot) \, d\Omega$ is the $L^2(\Omega)$-inner product. Equations (5.5) and (5.6) imply weak satisfaction of the momentum equations and the continuity equation, in addition to the initial condition.

**Remark:** The shape functions of linear tetrahedral elements are incomplete Lagrange polynomials that do not have cross terms. As a result, all the cross derivative are zero, and therefore they only cannot represent the cross terms of formulation (5.5)-(5.6). This makes tetrahedral elements behave in a stiff manner compared to hexahedral elements, which posses cross terms.

**Remark:** The objective in Sec. 5.3 is to develop a formulation for tetrahedral elements that is able to telescopically extract the smallest features of the solution of (5.5)-(5.6), and therefore, circumvent the limitations of tetrahedral elements.

### 5.3 The Variational Multiscale method

The variational multiscale framework assumes an overlapping additive decomposition of the unknown fields in the problem along with their weighting functions into coarse and fine scales [64, 95]. In the context of turbulence modeling, coarse scales represent the larger features in the flow. From a mathematical perspective, they belong to a finite dimensional
The fine scales, on the other hand, represent the higher modes on the wave-number axis as shown in Fig. 5.1, and they belong to an infinite dimensional space. Typically, the coarse scales are represented by the space of finite elements shape functions, and the fine scales are defined to be the remaining part of the solution. The key idea of the method is to model the fine-scale features either analytically or numerically, and then variationally project them onto the coarse-scale space. Consequently, the resulting coarse-scale problem has the effects of the fine scales uniformly represented via the variationally projected fine-scale model.

We assume a unique additive decomposition of the velocity field $v$ into coarse scales $\bar{v}$ and fine scales $v'$:

\[ v(x,t) = \bar{v}(x,t) + v'(x,t) \] (5.7)

We also decompose the pressure field into a coarse and a fine scale component denoted as $\overline{p}$ and $p'$, respectively:

\[ p(x,t) = \overline{p}(x,t) + p'(x,t) \] (5.8)

The spaces of functions for the coarse scales are defined to be linearly independent of the spaces used to represent the fine scales. For a detailed discussion on the spaces of functions see [64].

Similarly, we can assume an additive decomposition of the weighting functions of the velocity field $w$ and the pressure field $q$:

\[ w(x) = \overline{w}(x) + w'(x) \] (5.9)

\[ q(x) = \overline{q}(x) + q'(x) \] (5.10)

where $\overline{w}$ and $w'$ are the coarse and fine scale components of $w$, respectively, and $\overline{q}$ and $q'$ are the coarse and fine scale components of $q$, respectively.

**Remark:** In our previous work [98], we only assumed an overlapping multiscale decomposition of the velocity field $v$ and its weighting function $w$. In this work we
generalize the idea and also assume a multiscale decomposition of the pressure field $p$ and its weighting function $q$.

Substituting expressions (5.7)-(5.10) in the variational problem (5.5)-(5.6), and exploiting the linearity of the weighting functions, the weak problem can be decomposed in two sub-problems:

**Coarse-scale sub-problem:**

$$
\left( \frac{\partial (\bar{v} + v')}{\partial t}, (\nabla \bar{w}, (\bar{v} + v')) \right) - (\nabla \bar{w}, (\nabla (\bar{v} + v'))) + (\nabla ' \bar{w}, 2v ' (\bar{v} + v')) - (\nabla \cdot \bar{w}, p + p') - (\bar{w}, f) = 0
$$

$$
(q', \nabla \cdot (\bar{v} + v')) = 0
$$

**Fine-scale sub-problem:**

$$
\left( w', \frac{\partial (\bar{v} + v')}{\partial t} \right) - (\nabla w', (\nabla (\bar{v} + v'))) + (\nabla ' w', 2v ' (\bar{v} + v')) - (\nabla \cdot w', \bar{p} + p') - (w', f) = 0
$$

$$
(q', \nabla \cdot (\bar{v} + v')) = 0
$$

In the following section we first work on the fine-scales sub-problem with the objective of extracting the fine-scale solution from the problem (5.13)-(5.14) in terms of the residual of the Euler-Lagrange equations for the coarse scales. This is the modeling part of the method and provides options for representing the fine-scales with various levels of spatial and temporal sophistication. We then variationally embed the fine-scale model in the coarse-scale problem (5.11)-(5.12). This results in a formulation that only depends on the coarse scales, wherein the effects of the modeled fine scales are accounted for by the additional terms that emanate from the variational embedding of the fine-scale model.

**5.3.1 The mixed fine-scale problem: Modeling of the fine-scale fields**

Let us consider the fine-scale problem (5.13)-(5.14) which governs the evolution of the fine scales $v'$ and $p'$ in terms of the residuals of the coarse scales $\bar{v}$ and $\bar{p}$. Rearranging terms and applying integration by parts, problem (5.13)-(5.14) can be written in the following form:
\[(w', \frac{\partial v'}{\partial t}) + (w', v' \cdot \nabla \bar{v}) + (w', \bar{v} \cdot \nabla v')\]
\[+ (w', v' \cdot \nabla v') + (\nabla' w', 2\nu \nabla' v') - (\nabla \cdot w', p') = -(w', r_M)\]  
(5.15)

\[(q', \nabla \cdot v') = -(q', r_c)\]  
(5.16)

where

\[r_M = \frac{\partial \bar{v}}{\partial t} + \bar{v} \cdot \nabla \bar{v} - 2\nu \Delta' \bar{v} + \nabla \bar{p} - f\]  
(5.17)

is the residual of the Euler-Lagrange equations for momentum conservation and

\[r_c = \nabla \cdot \bar{v}\]  
(5.18)

is the residual of the continuity equation.

The objective at this point is to extract the fine-scale fields \(v'\) and \(p'\) from (5.15) and (5.16), which are infinite dimensional problems. In general, \(v'\) and \(p'\) cannot be exactly represented in terms of a finite dimensional sub-space. Consequently, simplifying assumptions need to be made in order to extract the fine-scale fields.

Since the fine-scale model attempts to capture the part of the solution that cannot be represented by the coarse scales, an order of magnitude analysis reveals that the norm of the coarse scale velocity is substantially larger than the norm of the fine-scale velocity. Consequently, the second order term \((w', v' \cdot \nabla v')\) can be neglected from (5.15). However, the second order term \((\bar{w}, v' \cdot \nabla v')\) that appears is (5.11) needs to be retained because it is known to be crucial for turbulence modeling [10].

To stabilize the fine-scale problem we apply the VMS framework to the mixed problem (5.15)-(5.16). This results in a further decomposition of the fine-scale, and thus yields a 3-level model. Figure 5.2 represents the hierarchical application of VMS ideas that result in a further decomposition of sub-grid scales into level-I and level-II scales. Figure 5.3 schematically shows the process of nesting of scales and the conceptual approach that is based on successive application of VMS ideas to solve the various scales involved in the problem. Accordingly, the coarsest scales, denoted by an overhead bar \((\bullet)\), represents the scales that the finite element discretization can capture. The fine scales, \((\bullet)'\), are further decomposed in two subsequent scales namely, the intermediate and the finest scales. The intermediate scales
also termed as fine-scales level-I and denoted by \((\bullet)_I'\), model the sub-grid features of the flow, and the finest scales, also called fine-scales level-II and denoted by \((\bullet)''_I\), are employed to stabilize the intermediate scales.

**Remark:** The fine-scale problem leads to a mixed formulation that involves the fine-scale fields \(v'\) and \(p'\), thus necessitating stabilization techniques to accommodate arbitrary discrete interpolations for \(v'\) and \(p'\). Consequently, we employ the VMS approach at the fine-scale level as well.

We assume a multiscale decomposition of the fine-scale velocity field \(v'\) and its weighting function \(w'\):

\[
v'(x,t) = v'_I(x,t) + v''_I(x,t)
\]

\[
w'(x) = w'_I(x) + w''_I(x)
\]  

In [97, 20, 98], we showed that a multiscale decomposition of the velocity field and its weighting function is enough to derive a stabilized formulation. Since in the present case the objective of applying the variational multiscale method to the mixed fine-scale-problem (5.15)-(5.16) is to enhance its stability property to be able to extract a stable fine-scale solution from it, we do not assume a multiscale decomposition of the fine-scale pressure field and its weighting function. Consequently,

\[
p'(x,t) = p'_I(x,t)
\]

\[
q'(x) = q'_I(x)
\]  

The interpolation spaces used to represent the intermediate scales and the finest scales must also be linearly independent to ensure consistency in the decomposition of problem (5.15)-(5.16).

Substituting the expressions (5.19)-(5.22) into (5.15)-(5.16), exploiting the linearity of the weighting slots, the fine-scale problem can be further decomposed in two sub-problems:
Fine-scale problem level-I:
\[
(w'^{I}, \frac{\partial (v'^{I} + v'^{II})}{\partial t} + (w'^{I}, (v'^{I} + v'^{II}) \cdot \nabla v) + (w'^{I}, \bar{v} \cdot \nabla (v'^{I} + v'^{II})) + (\nabla v'^{I}, 2v \nabla v) - (v \cdot w'^{I}, p'^{I}) = -(w'^{I}, r_{M})
\]
\[
(q'^{I}, \nabla \cdot (v'^{I} + v'^{II})) = -(q'^{I}, r_{C})
\]

Fine-scale problem level-II:
\[
(w'^{II}, \frac{\partial (v'^{I} + v'^{II})}{\partial t} + (w'^{II}, (v'^{I} + v'^{II}) \cdot \nabla v) + (w'^{II}, \bar{v} \cdot \nabla (v'^{I} + v'^{II})) + (\nabla v'^{II}, 2v \nabla v) - (v \cdot w'^{II}, p'^{I}) = -(w'^{II}, r_{M})
\]

As mentioned earlier, the fine-scale problem (5.15)-(5.16) is infinite dimensional, consequently, (5.23)-(5.25) are also infinite dimensional. At this point we need to make some simplifying assumptions to make the problem tractable. We therefore make an assumption that the fine scales vanish on the element boundaries:
\[
v' = w' = 0 \text{ on } \Gamma'
\]
\[
p' = q' = 0 \text{ on } \Gamma'
\]
where \(\Gamma'\) is the union of element boundaries. Although this simplification is not strictly necessary, it is convenient to localize the solution of the fine-scale problem to element interiors or to patches of elements. This facilitates the design of fine-scale models that are computationally economical and amenable to parallel implementation. For consistence with (5.26)-(5.27), the intermediate scales and the finest scales are chosen to vanish on the element boundaries as well. For instance, the intermediate scales can be represented by quadratic bubble functions and the finest scales by fourth order polynomial bubbles.

5.3.1.1 Modeling of the fine-scales level-II

We will now extract the velocity \(v_{II}\) from problem II in terms of the residual \(r_{M}\) and the intermediate scales. Rearranging the terms in (5.25), problem II can be written as:
\[(w'_H, \partial v'_H/\partial t) + (w'_H, v'_H, \nabla) + (w'_H, \bar{v}, \nabla v'_H) + (\nabla^I w'_H, 2v\nabla^I v'_H)\]
\[= - (w'_H, r_M) - (w'_H, \partial v'_I/\partial t) - (w'_H, v'_I, \nabla) - (w'_H, \bar{v}, \nabla v'_I)\]
\[- (\nabla^I w'_H, 2v\nabla^I v'_I) + (\nabla \cdot w'_H, p'_I)\]

(5.28)

We express the variables \((*)_H\) in terms of bubble functions that are polynomial functions and vanish on the element boundaries as expressed in the conditions (5.26)-(5.27):

\[v'_H = \beta b'_H\quad \text{in } \Omega^e\]
\[w'_H = \gamma b'_H\quad \text{in } \Omega^e\]

(5.29) (5.30)

where \(\beta\) and \(\gamma\) are the element internal unknowns that scale the bubble function \(b'_H\).

Equation (5.28) can be discretized in time using any time integrator for the first-order systems. We employ the generalized-alpha method [70] in which the terms in (5.28) that contain time derivatives are evaluated at time level \(n+\alpha_m\) and the other terms at \(n+\alpha_f\), where \(\alpha_m\) and \(\alpha_f\) are correlated parameters. Thus,

\[\left(v'_H\right)_{n+\alpha_f} = \left(v'_H\right)_n + \alpha_f \left(\left(v'_H\right)_{n+1} - \left(v'_H\right)_n\right)\]

(5.31)

\[\left(\partial v'_H/\partial t\right)_{n+\alpha_m} = \left(\partial v'_H/\partial t\right)_n + \alpha_m \left(\left(\partial v'_H/\partial t\right)_{n+1} - \left(\partial v'_H/\partial t\right)_n\right)\]

(5.32)

The generalized-alpha method also enforces

\[\left(v'_H\right)_{n+1} = \left(v'_H\right)_n + \Delta t \left(\partial v'_H/\partial t\right)_n + \Delta t \gamma \left(\left(\partial v'_H/\partial t\right)_{n+1} - \left(\partial v'_H/\partial t\right)_n\right)\]

(5.33)

where \(\gamma = 1/2 + \alpha_m - \alpha_f\).

Substituting (5.29)-(5.33) in (5.28), integrating by parts the last two terms on the right hand side of (5.28), retaining the mean value of the residual over the element interiors, and dropping the contribution of time-history terms, the fine scale level-II component of the velocity field can be expressed as:

\[v'_H = - \tau_H (r_M + v'_I, \nabla \bar{v} + \bar{v}, \nabla v'_I - 2v \Delta v'_I + \nabla p'_I)\]

(5.34)
Remark: Equation (5.34) shows that there is spatio-temporal coupling between the coarse and fine scales because the residual at level-II is a function of the coarse solution \( \{ \mathbf{v}, p \} \) as well as the fine-scale level-I solution \( \{ \mathbf{v}_I', p_I' \} \). This is an important ingredient of the two-way coupling facilitated by the multiscale method presented here.

In (5.34), the variational projector that embeds \( \mathbf{v}_I' \) into the variational equation at level-I is defined as

\[
\tau_{II} = b_{II}^c \left\{ \frac{\alpha_m}{\gamma} \int_{\Omega_e} (b_{II}^c)^2 \mathrm{d}\Omega + \alpha_f \hat{\mathbf{t}} \right\}^{-1}
\]

in which \( \Delta t \) is the time step size; \( \alpha_m, \alpha_f \) and \( \gamma \) are the parameters of the time-integration scheme, which in the present case is the generalized-alpha method. In this derivation a definition of \( \hat{\mathbf{t}} \) emerges

\[
\hat{\mathbf{t}} = \int_{\Omega_e} \left( b_{II}^c \right)^2 \nabla^T \mathbf{v} \mathrm{d}\Omega + \int_{\Omega_e} b_{II}^c \mathbf{f} \cdot \nabla b_{II}^c \mathrm{d}\Omega \mathbf{I} + \int_{\Omega_e} \nabla |\nabla b_{II}^c|^2 \mathrm{d}\Omega \mathbf{I} + \nabla \int_{\Omega_e} \nabla b_{II}^c \otimes \nabla b_{II}^c \mathrm{d}\Omega
\]

which is a second order tensor that is form analogous to the tensor valued \( \hat{\mathbf{t}} \) derived in [98]. It is well documented that the skew advection term vanishes if the same bubble function is used to interpolate both \( \mathbf{v}_I' \) and \( \mathbf{w}_I' \). To retain the contribution of this term, and thus to account for the sharp advection layers in the level-II scales, we employ the method presented in [97] that utilizes ideas from the residual free bubbles method [17] and modifies the bubble function that is used in the weighting slot of the skew advection term.

Remark: In the derivation of (5.34) we have assumed that the finest scales are quasi-static, and we have dropped the contribution from their time-history terms. Due to the iterative nature of the problem, this amounts to making a first order approximation in time for the fine scales. However, we have kept the dependence of the time step size in the definition of \( \tau_{II} \) which is facilitated by the first term in (5.35).
Remark: The functional form of (5.36), which is similar to [98], is a consequence of the homogeneous multiscale approach [99] because the same differential equation is assumed to govern the physics at the various levels of the problem description.

5.3.1.2 Modeling of the mixed field problem at level-I

\[
\left( w'_{I}, \frac{\partial v'_{I}}{\partial t} \right) + \left( w'_{I}, v'_{I} \cdot \nabla \overline{v} \right) + \left( w'_{I}, \overline{v} \cdot \nabla v'_{I} \right) + \left( \nabla' w'_{I}, 2 \nu \nabla' v'_{I} \right) \\
- \left( \nabla \cdot w'_{I}, p'_{I} \right) + \left( q'_{I}, \nabla \cdot v'_{I} \right) \\
- \left( w'_{I} \cdot \nabla' \overline{v} - \overline{v} \cdot \nabla w'_{I} - 2 \nu \Delta' w'_{I} - \nabla q'_{I}, \tau_{H} \left( v'_{I}, \nabla' \overline{v} + \overline{v} \cdot \nabla v'_{I} - 2 \nu \Delta' v'_{I} + \nabla p'_{I} \right) \right) \\
= - \left( w'_{I}, r_{M} \right) - \left( q'_{I}, r_{C} \right) \\
+ \left( w'_{I} \cdot \nabla' \overline{v} - \overline{v} \cdot \nabla w'_{I} - 2 \nu \Delta' w'_{I} - \nabla q'_{I}, \tau_{H} r_{M} \right) \\
\tag{5.37}
\]

Equation (5.37) presents a mixed field problem with embedded stabilization terms that have been consistently derived employing the VMS framework. Because of the stabilization features, arbitrary combinations of interpolation functions can now be used to solve problem (5.37). To solve (5.37), we interpolate the fine-scale level I fields using bubble functions \( b_{I}^{e} \), where the same bubble interpolation is employed to represent the velocity and pressure fields:

\[
\begin{pmatrix}
    v'_{I} \\
    p'_{I}
\end{pmatrix} = \alpha \ b_{I}^{e} \\
\begin{pmatrix}
    w'_{I} \\
    q'_{I}
\end{pmatrix} = \delta \ b_{I}^{e} \\
\tag{5.38}
\]

where \( \alpha \) and \( \delta \) are the coefficients of the variables that are used to represent the intermediate fields.

Remark: To fulfill the condition of linear independence between the spaces of functions for fine-scales level-I and level-II, the bubble functions \( b_{I}^{e} \) and \( b_{II}^{e} \) must be linearly independent. For instance, \( b_{I}^{e} \) can be a quadratic bubble and \( b_{II}^{e} \) a fourth order polynomial bubble.

Remark: The VMS framework applied to the fine-scale problem (5.15)-(5.16) addresses two numerical instabilities that arise (i) due to the reason that the problem is a mixed field problem, and (ii) due to the issues related to the advection term. Therefore, the VMS-
stabilized fine scale formulation (5.37) can be solved employing the same bubble function \( b_f \) in all the terms, and due to the additional stabilization terms, the resulting model represents well all the physics of the problem.

Substituting (5.38)-(5.39) in (5.37) and applying the generalized-alpha method, the fine-scale level-I problem becomes

\[
\left( \frac{\alpha_m}{\Delta t \gamma} \ddot{M} + \alpha_f \ddot{K} \right) \alpha_{n+1} = R - \alpha_m \frac{\gamma-1}{\gamma} \dot{M} \hat{\alpha}_n + \frac{\alpha_m}{\Delta t \gamma} \ddot{M} \alpha_n - (1 - \alpha_f) \dot{K} \alpha_n \tag{5.40}
\]

where \( \dot{M} \) is the matrix that is obtained when the interpolations (5.38)-(5.39) are substituted into the mass terms of (5.37). The vector \( R \) contains all the terms of (5.37) that depend on the residual of the Euler-Lagrange equations for the coarse-scales \( r_M \) and \( r_C \). Finally, \( \dot{K} \) is the matrix that encompasses the remaining terms. As was the case in level-II problem, any time integration scheme can be used for the present level-I problem as well. However, for clarity of presentation, we have used the same time integration scheme here. Furthermore, the same time step size \( \Delta t \) is also used to advance the level-I scales in time.

Combining (5.38) and (5.40), the level-I solution can be expressed as:

\[
\begin{bmatrix}
\dot{v}'_I \\
\dot{p}'_I
\end{bmatrix}_{n+1} = - b_f^e \tau \begin{bmatrix}
r'_M \\
r'_C
\end{bmatrix}_{n+\alpha_f} + \mathcal{F}(v'_I, p'_I)|_n
\tag{5.41}
\]

where the terms in (5.40) that depend on \( \alpha_n \) and \( \dot{\alpha}_n \) have been grouped in the functional \( \mathcal{F} \) which is defined as

\[
\mathcal{F}(v'_I, p'_I)|_n = b_f^e \left( \frac{\alpha_m}{\Delta t \gamma} \ddot{M} + \alpha_f \ddot{K} \right)^{-1} \left[ -\alpha_m \frac{\gamma-1}{\gamma} \dot{M} \hat{\alpha}_n + \frac{\alpha_m}{\Delta t \gamma} \ddot{M} \alpha_n - (1 - \alpha_f) \dot{K} \alpha_n \right]
\tag{5.42}
\]

The functional \( \mathcal{F} \), evaluated at time step \( t_n \), contains all the time-history terms of the fine-scales level-I. The other term that contributes to fine-scales level-I in (5.41) depends on the residuals of the coarse scale momentum and continuity equations, \( r_M \) and \( r_C \), respectively evaluated at time level \( t_{n+\alpha_f} \).
In (5.41), the first term on the right hand side is driven by the residual of the coarse scales, and the second order tensor $\tau$ is obtained by inverting the matrix

$$\left( \frac{\alpha_m}{\Delta t} \hat{M} + \alpha_f \hat{K} \right),$$

multiplying it by $R$ and assuming a constant projection of $r_M$ and $r_c$ over element interiors.

It is important to note that we have employed a nested VMS framework between level-I and level-II fine scale modeling. Consequently embedding $v''_{II}$ into level-I mixed problem, and modeling of $\{v', p'_{I}\}$ in a residual form actually leads to $\{v', p'_{I}\}$ with embedded $v''_{II}$, i.e., $\{v'_{I}(v''_{II}), p'_{I}(v''_{II})\}$. Therefore, comparing with equation (5.19), and considering that $v''_{II}$ is only used to stabilize the level-I problem, we can replace the right hand side of (5.19) via the modified level-I fine scale with embedded level-II fine scale. Consequently, we set

$$\begin{pmatrix} v'_I \\ p'_I \end{pmatrix}_{n+1} = \begin{pmatrix} v'_I \\ p'_I \end{pmatrix}_{n+1}$$

(5.43)

5.3.1.3 **Modeling simplifications for the fine-scale variational operator**

In order to design computationally economic turbulence models several modeling simplifications can be applied. The $4 \times 4$ second order tensor $\tau$ that arises from the solution of the linearized system of equations is, in general, non-diagonal. The model (5.41) can be simplified by only considering the diagonal terms of $\tau$. This leads to substantial computational economy in the computation of the fine scales. In Sec. 5.4 we will show by means of a numerical test that the off-diagonal terms do not have a significant effect on the computed solution of the turbulent channel flow. Nevertheless, there are some problems with strong cross-wind coupling effects where off-diagonal terms in $\tau$ may actually enhance the stability of the formulation. There have been some recent efforts in the literature to design stabilization parameters $\tau$ that possess off-diagonal terms, and thus bring cross-wind coupling [122]. In our work, the off-diagonal terms are derived naturally via the solution of the fine-scale problem.
The model defined in (5.41) is time dependent, and therefore the time history variables need to be stored at the points where the solution is to be evaluated (i.e., Gauss points). For large meshes, keeping track of the time history at Gauss points in every element is a memory intensive task. The proposed model can be simplified by neglecting the time-history of the fine scales but retaining the dependence of $\tau$ on the time step size $\Delta t$.

In the numerical test section our baseline formulation will be the one that employs the diagonalized $\tau$ and also neglects the contribution of the time-history of the fine scales, i.e., the functional $\mathcal{F}(v_I, p_I)|_{\Omega}$ in equation (5.41).

**Remark:** Neglecting the off-diagonal terms of the $4 \times 4$ second order tensor $\tau$ decouples the solution of the fine-scale velocity and pressure fields, and simplifies significantly the computational cost of the model.

**Remark:** For the sake of simplicity, we have used the same time integration scheme for the coarse-scale problem and the two fine-scale problems. Thus, the time step size $\Delta t$ to be used is taken to be the one that is able to resolve the temporal scales in all the three problems. Nevertheless, this is not a concern because in the numerical tests section we obtain accurate results using the same time step size as the ones published in the literature for similar problems.

**Remark:** In some physical problems, the optimal time step size for the coarse scales may not be small enough to accurately resolve the finer scales. In these cases, the time step size needs to be adapted to a size that accurately solves all the scales. This constraint on the time step size can be relaxed by employing multi-stepping techniques, or using a higher order accurate time integration schemes for the fine-scales problems that have higher frequencies.

**Remark:** In [98] we solved the fine-scale problem using ideas from the residual free bubbles method [17]. In the present Chapter we make minimum possible assumptions in the modeling of the fine-scales level-I to model to make the problem finite dimensional and therefore tractable. The required simplifications are done only at the fine-scales level-II. This yields an enhanced formulation that is robust in the representation of fine scale effects and successfully
compensates for the inherent stiff response of low order tetrahedra in unstructured tetrahedral meshes.

### 5.3.2 Residual-based turbulence model

The fine-scale solution obtained in Sec. 5.3.1 can be embedded in the coarse-scale problem (5.11)-(5.12). Since the fine-scale models are in fact driven by the coarse-scale fields via the residual equations, the resulting formulation can be expressed in terms of the coarse scales $\tilde{v}$ and $\tilde{p}$. Combining equations (5.11) and (5.12) and integrating by parts the terms that contain spatial derivatives of the fine scales, the coarse-scale problem is re-written as follows:

$$
(\tilde{w}, \frac{\partial \tilde{v}}{\partial t}) - (\nabla \tilde{w}, \tilde{v} \otimes \tilde{v}) + (\nabla' \tilde{w}, 2\nu \nabla' \tilde{v}) - (\tilde{v} \cdot \nabla \tilde{w}, p) + (q, \nabla \cdot \tilde{v}) \\
+ (\tilde{w}, \frac{\partial \tilde{v}'}{\partial t}) - (\tilde{v} \cdot \nabla \tilde{w} + \tilde{v} \cdot \nabla' \tilde{w} + \nabla \tilde{q} + 2\nu \Delta \tilde{w}, \tilde{v}') \\
- (\nabla \tilde{w}, \tilde{v} \otimes \tilde{v}') - (\nabla \cdot \tilde{w}, \tilde{p}') \\
= (\tilde{w}, f)
$$

(5.44)

In (5.44) we can identify the standard Galerkin terms $B_{\text{Gal}}(\tilde{w}, \tilde{q} ; \tilde{v}, \tilde{p})$ and $F_{\text{Gal}}(\tilde{w})$ that were present in the standard weak form (5.5)-(5.6):

$$
B_{\text{Gal}}(\tilde{w}, \tilde{q} ; \tilde{v}, \tilde{p}) = (\tilde{w}, \frac{\partial \tilde{v}}{\partial t}) - (\nabla \tilde{w}, \tilde{v} \otimes \tilde{v}) + (\nabla' \tilde{w}, 2\nu \nabla' \tilde{v}) \\
- (\nabla \tilde{v} \cdot \tilde{w}, p) + (\tilde{q}, \nabla \cdot \tilde{v}) \\
(5.45)

F_{\text{Gal}}(\tilde{w}) = (\tilde{w}, f)

(5.46)

Equation (5.44) also contains some additional terms, namely

$$
B_{\text{VMS}}^{\text{Turb}}(\tilde{w}, \tilde{q} ; \tilde{v}, \tilde{v}', p') = (\tilde{w}, \frac{\partial \tilde{v}'}{\partial t}) - (\tilde{v} \cdot \nabla \tilde{w} + \tilde{v} \cdot \nabla' \tilde{w} + \nabla \tilde{q} + 2\nu \Delta \tilde{w}, \tilde{v}') \\
- (\nabla \tilde{w}, \tilde{v} \otimes \tilde{v}') - (\nabla \cdot \tilde{w}, \tilde{p}')
$$

(5.47)

that variationally project the effects of the fine scales onto the coarse-scale space and thus provide a consistently derived residual-based turbulence model.

The residual-based turbulence model (5.44) can be expressed in an abstract form as

$$
B_{\text{Gal}}(\tilde{w}, \tilde{q} ; \tilde{v}, \tilde{p}) + B_{\text{VMS}}^{\text{Turb}}(\tilde{w}, \tilde{q} ; \tilde{v}, \tilde{v}', p') = F_{\text{Gal}}(\tilde{w})
$$

(5.48)
Remark: In our previous work [98], we did not perform a split of the pressure field and assumed the fine scale pressure \( p' = 0 \). Instead we injected a term proportional to \( \nabla \cdot \overline{v} \) in the final formulation, and numerical tests showed that better conservation of mass is achieved if the pressure stabilization term is taken into account. In the present formulation, we have performed a split of the pressure field in (5.8) and a fine scale pressure field automatically leads to a pressure stabilization term.

Remark: A key feature of the proposed formulation is that it can be easily implemented in existing finite element codes. The only parts that need to be modified are the functions that compute the element consistent tangent matrices \( (K^f)^n_i \) and the element residual vectors \( (R^f)^n_i \), where \( i \) and \( n \) are the non-linear iteration and the time step counters, respectively. The algorithm to solve the fluid flow problem using the proposed method is outlined in Box 5.1.

Remark: To keep the presentation simple and easy to follow, Box 1 describes the algorithm for the turbulence model that ignores the time-history of the fine scales, i.e. ignores the contribution \( \mathcal{F} \) of in eq. (5.41). If time-dependence of fine scales is to be included, then fine-scale level-I variables need to be updated at steps 1, 3, 9 and 11 using the full expression given in equation (5.41).

Remark: Tangent matrix \( (K^f)^n_i \) and residual vector \( (R^f)^n_i \) can be easily implemented in a finite element code using the guidelines outlined in Appendix A.

5.4 Numerical results

Most of the existing turbulence models are suitable for structured meshes. However, domain discretizing schemes that are based on unstructured tetrahedral elements are very convenient for discretizing domains with complex geometries. Therefore, turbulence models that are accurate for tetrahedral elements have a great potential to be used in industrial strength problems. In Sec. 5.3 we have presented a residual-based turbulence model for unstructured tetrahedral meshes. The new model is based on a sophisticated treatment of fine scales with the least number of modeling assumptions, thereby adding to the flexibility of the
tetrahedral elements to model the sub-grid scale physical phenomena, thus yielding a LES model for tetrahedral elements. In the present section, we employ two numerical tests to study the accuracy of the proposed formulation and the effects of some of the modeling assumptions and simplifications adopted in the development of the fine-scale model. We first consider a turbulent channel flow at \( \text{Re}_T = 395 \) and \( \text{Re}_T = 590 \). We compare the proposed method for tetrahedral meshes with the reference DNS solution [103] and the results obtained with other VMS methods [10]. We also compare the present results with the model presented in [98] for hexahedral meshes. In addition, we study the effect of diagonalizing the operator \( \tau \) that appears in the derivation of the fine-scale models. We also study the effect of simplifying the time dependence of fine scales.

The second problem is flow around an airfoil SD-7003 at \( \text{Re} = 60,000 \) and an angle of attack \( \alpha = 4^\circ \). This flow is more complex because at the leading edge of the airfoil the flow is laminar and after a transition zone it becomes turbulent in the proximity of the trailing edge. Additionally, on the upper surface of the airfoil the boundary layer detaches and then reattaches at a downstream point. We compare our results with the experimental results [107] and the numerical results obtained by Uranga et al. [130] and Galbraith and Visbal [42] for a compressible fluid at low Mach number. We also include the results obtained using the model presented in [98] for hexahedral meshes.

The numerical tests have been performed using linear and quadratic (see Fig. 5.4) tetrahedral elements. To evaluate the fine-scale level-I fields, we have used quadratic polynomial bubble functions, and to evaluate the tensor used to stabilize the fine-scale problem, we have used fourth-order bubble functions along with the skew-bubble proposed in [97]. The time integration scheme chosen is the generalized alpha method, and its parameter \( \rho_\alpha \) is set to 0. For the evaluation of element level integrals, full integration rule has been employed.

5.4.1 Turbulent channel flow

Turbulent channel flow is a typical benchmark problem for turbulence models because well-established reference DNS solutions are available [103]. We study the channel flow at \( \text{Re}_T = 395 \) and \( \text{Re}_T = 590 \) using different resolution meshes of tetrahedral elements and we
compare the results with the reference DNS solution. We also compare our results with other VMS results [10] and the results obtained with hexahedral meshes using a previous model for the fine scales [98]. Figure 5.5 shows the schematic diagram of the channel problem. No-slip boundary conditions are applied at the walls that are normal to the y-direction. On all the other faces, periodic boundary conditions are applied. The flow is driven by a body force \( f_x \) applied in the x-direction. For the lower Reynolds number flow, we set \( f_x = 0.00337204 \) and \( \nu = 0.0001472 \), and the dimensions of the channel are \( 2 \pi \) in the x-direction, 2 in the y-direction and \( (2/3) \pi \) in the z-direction. For the second flow that corresponds to \( Re_T = 590 \), the flow parameters are \( f_x = 1.0 \) and \( \nu = 0.001694915 \), and the dimensions are \( 2 \pi, 2 \) and \( (2/3) \pi \) in the x, y and z-directions, respectively. In all the cases, the flow is initialized with a perturbed parabolic velocity profile and zero pressure as the initial condition. The flows are let to evolve until they reach a statistical steady state regime. Then, 5,000 additional time steps are computed to extract the main statistical characteristics of the flow. The time step size \( \Delta t \) is set to 0.025 and 0.0015 for \( Re_T = 395 \), and \( Re_T = 590 \), respectively. For the cases where other time step sizes are employed, \( \Delta t \) is clearly specified in the corresponding numerical test description.

All the meshes employed here have nodal points evenly spaced in the x and z-directions, and they are distributed in the y-direction according to the following hyperbolic function:

\[
y_i = -\frac{\tanh(\gamma(1-2i/(N-1)))}{\tanh(\gamma)}
\]  

(5.49)

where \( y_i \) is the nodal coordinate in the y-direction, \( i \in [0,N-1] \), \( N \) is the total number of nodal points in the y-direction and \( \gamma \) is a parameter which is set to 2.75 for all the numerical tests.

First we consider the flow at \( Re_T = 395 \), which is solved using a mesh that consist of 196,608 linear tetrahedral elements, and a second mesh with 24,576 10-node tetrahedral elements. Both meshes have \( 32 \times 33 \times 32 \) nodes, which are distributed in a similar manner. Figure 5.6 shows the mean stream-wise velocity \( U^+ \) and the root mean square fluctuations in
the $x$, $y$ and $z$ directions, which are denoted as $u^+$, $v^+$ and $w^+$, respectively. The plots also show the results obtained with a VMS method using linear hexahedral elements [10], and the results obtained with a hexahedral mesh using the turbulence model presented in [98]. For both cases the mesh is comprised of $32 \times 32 \times 32$ elements. Also shown is the reference DNS solution [103] which was obtained employing a grid of $384 \times 258 \times 384$ points. Figure 5.6 shows that the results obtained with 4-noded tetrahedra using the turbulence model presented in Sec. 5.3 are almost as accurate as the results obtained with equivalent meshes consisting of 8-noded hexahedra. Since low order tetrahedra are very simple (i.e., they do not have bi-linear, tri-linear or higher-order terms), the accuracy obtained indicates that the fine-scale model presented here is effective in compensating the overly stiff effects usually associated with linear tetrahedral. The results obtained with 10-node tetrahedral elements are more accurate than the results obtained with the hexahedral mesh for the same number of degrees of freedom.

Figure 5.7 shows a similar study but performed with refined meshes that consist of $64 \times 65 \times 64$ nodal points that constitute 1,572,864 linear tetrahedral elements and 196,608 quadratic tetrahedral elements. The results obtained with the 10-node elements are clearly more accurate. For comparison proposes, Fig. 5.7 also shows the results obtained with the formulation presented in [98] for 262,144 linear hexahedral elements and the reference DNS solution [103].

Figure 5.8 shows a similar study performed for $Re_T = 590$, employing meshes consisting of $64 \times 65 \times 64$ nodal points, comprising 1,572,864 linear tetrahedral elements, or 196,608 quadratic tetrahedral elements. Also shown are the results for the mesh that comprises 262,144 linear hexahedral elements that were obtained with the formulation proposed in [98]. The reference DNS results reported in [103] were obtained with a $384 \times 258 \times 384$ points grid. A similar trend as in the previous test case is seen. The performance of linear tetrahedral elements is analogous to that of the linear hexahedral elements. Furthermore, the results obtained with the 10-node tetrahedral elements are uniformly better than that of the linear elements, thus highlighting the $p$-refinement feature of the residual-based turbulence model.
5.4.1.1 Effects of diagonalizing the fine-scale operator

The tensor $\tau$ that appears in the derivation of the fine-scale model presented in Sec. 5.3 is a $4 \times 4$ second order tensor. With an objective of developing a computationally economic model for the fine scales, we propose to omit the off-diagonal values in $\tau$. This simplification results in a reduction in the cost of computation of the fines scales, and therefore in the formation of the systems of linearized equations. In this section we employ the channel flow problem to analyze the effects of this modeling assumption on the computed results. Figure 5.9 compares the results obtained with the full model, i.e. the full non-diagonal $\tau$, and the diagonalized model for the case of $Re_T = 395$. Also presented are the DNS results. Employing 10-node tetrahedral with the mesh of $32 \times 33 \times 32$ nodal points, the results obtained from both models are almost the same. This means that the diagonalization of $\tau$ is a modeling assumption that does not affect significantly the resulting fine-scale model.

5.4.1.2 Time dependency of the fine-scale model

Section 5.3 presents different models for the fine-scales with various modeling simplifications considered in the spatial and temporal domains. In this section we study the effect of the modeling simplifications that can be done with regard to the temporal domain. A very economical fine-scale model can be obtained if the time history of the fine scales is omitted. Although this simplification ignores the history terms, the model retains dependence on the time step size $\Delta t$. In the present section we perform a time step size refinement to study the behavior of the simplified fine-scale model and the behavior of the model that retains the full time dependences of the fine scales.

We consider the $Re_T = 395$ channel problem and discretize the domain using a mesh with 24,576 quadratic tetrahedral elements, comprising $32 \times 33 \times 32$ nodal points. We employ three time step sizes: $\Delta t = \Delta t_1 = 0.025$, $\Delta t = \Delta t_1 / 4 = 0.00625$ and $\Delta t = \Delta t_1 / 16 = 0.0015625$.

In [98], we proposed an earlier version of fine-scale model that omitted the time history of fine scales. A similar time step size study resulted in most accurate results for $\Delta t = \Delta t_1$ above. A dramatic reduction in the accuracy of the solution was observed for the case of $\Delta t = \Delta t_1 / 4$, and we were not able to get results for the case for substantially finer time step sizes. This degradation in accuracy is attributed to the fact that as $\Delta t \to 0$ the fine scales
also tend to vanish, and therefore the simplified fine-scale model presented in [98] is not able to stabilize the formulation and take into account of the sub-grid effects for very small time step sizes.

Figure 5.10 shows the results obtained with the present model that omits the time dependence of the fine scales. Still the accuracy is comparable for the three time step sizes. Although the model that ignores time history also vanishes as $\Delta t \to 0$, it is still more robust than the one presented in [98] and can be applied to accurately solve turbulent flows for a wider range of time step sizes.

Figure 5.11 shows the time step size study in which the model that takes into account the full temporal evolution of the fine scales is used. The model delivers same accuracy for all the three time steps employed.

5.4.2 Turbulent flow around an airfoil

The proposed method can be applied to study fluid flows in a wide range of engineering applications. An important area of application is the aircraft industry, where robust turbulence modeling methods can be used to design and analyze aircraft structures.

In this section, we consider a prismatic airfoil SD-7003 of infinite width and unit chord $c$. The computational domain is represented in Fig. 5.12, where it can be seen that the lateral and outflow boundaries are located 6 units apart from the airfoil. The upstream boundary is a circular arch of radius 6 units with center located at the trailing edge of the airfoil. In the span-wise direction, the computational domain is extended over 0.2 units. A unit inflow velocity with an angle of attach $\alpha$ of $4^o$ is prescribed on the lateral and circular boundaries, and periodic boundary conditions are specified in the span-wise direction. The viscosity $\nu$ is set to $1/60,000$. Thus, the Reynolds number based on the inflow velocity and the chord of the airfoil is 60,000. The problem is initialized from at rest state at $t = 0$ and the inflow velocity is gradually increased at a constant rate until it reaches the maximum magnitude at $t = 5$. Then, the flow is let to develop and evolve until $t = 25$.

The domain is discretized using one mesh of tri-linear hexahedral elements and two meshes of quadratic tetrahedral elements. All the meshes have been obtained extruding bi-dimensional meshes in the z-direction. The hexahedral mesh consists of 458,784 nodes spread
through 16 layers and it has a total number of 452,480 hexahedral elements. The nodes closest to the surface of the airfoil are spaced $7.8 \times 10^{-4}$ in the normal direction to the surface. The coarsest quadratic tetrahedral meshes consist of 1,290,784 nodes and 1,921,920 elements and the finest mesh has 1,913,496 nodes and 2,850,120 elements. The coarse mesh has 22 layers of nodes while the finest mesh has 26 layers. The spacing of the nodes in the normal direction to the airfoil surface is $5.85 \times 10^{-4}$ and $5.1 \times 10^{-4}$ for the coarsest and finest meshes, respectively. Figure 5.13 shows the details of the coarse tetrahedral mesh on the vicinity of the airfoil. The time step sizes employed are $\Delta t = 0.005$ and $\Delta t = 0.0025$.

The fully developed flow is still laminar on the lower side of the airfoil. On the upper side, the boundary layer detaches from the airfoil and the flow transitions to a turbulent regime. In the statistically averaged flow, a laminar separation bubble forms on the upper side of the airfoil. The transitional behavior of the flow can be observed in Fig. 5.14(a), which shows q-criterion iso-surfaces and velocity streamlines. Figure 5.14(b) shows a close up view of the streamlines near the region where the boundary layer detaches from the airfoil.

The solution fields are sampled every 5 time steps starting at $t = 15$ and until the computations reach the final time at $t = 25$. Then the samples are averaged over time and over the span-wise direction. Figure 5.15 shows a color map of the averaged velocity field and velocity streamlines, which show the presence of a laminar separation bubble on the upper side of the airfoil.

The computed statistics of the flow are compared to the results obtained numerically in [42] and [130] and the experimental results reported in [107]. In these cases, the flow was considered compressible. Since in the present problem the Mach number is low, the effects of the flow compressibility are small, and thus the previously reported results provide a good reference for comparison with the present results that have been obtained with the method with embedded incompressibility. Table 5.1 shows the characteristics of the laminar separation bubble. In addition to the experimental data and the previously published numerical results, the table also shows the results obtained employing (i) the hexahedral element meshes and the coarse tetrahedral meshes with $\Delta t = 0.005$, and (ii) the results obtained using the finest tetrahedral mesh. For the finest mesh, two time step sizes are employed, i.e. $\Delta t = 0.0025$ and $\Delta t = 0.005$, to show that the results are insensitive to the time
step size refinement. In all the tests we see a good agreement with the previously published results. Figures 5.16 and 5.17 show the mean pressure coefficient and the mean drag coefficient, respectively. Each of the figures has two branches that correspond to the upper and lower surfaces of the airfoil. In all the cases, computed results agree very well with the published results.

5.5 Conclusions

We have presented a residual-based turbulence model for unstructured tetrahedral meshes. The method is derived via a telescopic application of the VMS ideas. In the present work, the sub-grid scales are fully time-dependent and are derived via the solution of a mixed field problem, which has also been stabilized via the VMS method. This three scale nested formulation provides a consistent top-down and bottom-up linking of scales, thus yielding a sophisticated platform for refined representation of fine scales. The coarse scales are associated with the larger features in the flow and can be captured using the finite element discretization. The intermediate scales serve as the refined turbulence model in addition to facilitating the stabilization of the problem governing the coarse scales. Lastly the fine scales are there to stabilize the mixed problem that governs the intermediate scales.

The solution of the fine-scale problem belongs to an infinite dimensional space, and thus obtaining the exact solution is not feasible in most cases. Consequently, some modeling assumptions need to be made to make the problem finite dimensional. In the proposed method, most of these modeling assumptions have been done at the finest level, i.e., fine-scale level-II. Thus a reduced number of assumptions on the fine-scales at level-I serves as a sophisticated and refined residual-based turbulence model that is accurate for unstructured tetrahedral meshes. The proposed method provides a powerful tool to study problems that are discretized with tetrahedral elements because these elements provide flexibility to discretize domains with complex geometries, such as the ones typically encountered in most industrial strength problems.

We have shown the accuracy of the proposed formulations via two benchmark problems. The first problem is the turbulent channel flow, which has been solved for $Re_T = 395$ and $Re_T = 590$. The solutions obtained with linear tetrahedral element are comparable to the solution obtained via our previous formulation using hexahedral elements.
For an equivalent number of degrees of freedom, the results obtained with quadratic tetrahedral elements are more accurate than the two linear element types. This is due to the fact that quadratic elements can better represent the terms that include second spatial derivatives. We have also employed the turbulent channel flow to study some of the modeling simplifications that can be adopted in the derivation of the turbulence models for computational economy. In particular, we have shown that the diagonalization of the tensor $\tau$, which reduces the computational cost, does not affect the solution significantly. The effects of neglecting the time history of the fine scales have also been studied. For analogous model presented in [98], in which time history terms were neglected, a dramatic loss of accuracy was observed for very small time steps sizes. This is attributed to the vanishing behavior of the fine-scale models as the time-step size is decreased. In the present model we have observed improved accuracy in the small time-step range because of the sophisticated treatment of the fine-scales.

The second problem that we have studied is the flow around a prismatic airfoil at $Re = 60,000$. We have compared our results with the results reported by Uranga and co-workers [130], Galbraith and co-workers [42] and Ol and co-workers [107] and good agreement has been observed. This second test problem has shown the accuracy and applicability of the formulation for more complex fluid flows.

### 5.6 Figures, boxes and tables

![Figure 5.1 Conceptual decomposition of the solution fields in coarse- and sub-grid scales](image)
Figure 5.2 Conceptual decomposition of the scales along the wavelength axis

Figure 5.3 Schematic diagram of telescopic depth in scales approach
Figure 5.4 (a) Linear and (b) quadratic tetrahedral elements

Figure 5.5 Schematic representation of the channel
Figure 5.6 Statistics of the turbulent channel flow at Re=395 obtained with the coarse mesh. (a) Mean stream-wise velocity. RMS velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 5.7 Statistics of the turbulent channel flow at Re=395 obtained with the fine mesh. (a) Mean stream-wise velocity. RMS velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 5.8 Statistics of the turbulent channel flow at Re=590. (a) Mean stream-wise velocity. RMS velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 5.9 Effects of the diagonalization of the fine-scale operator. (a) Mean stream-wise velocity. RMS velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 5.10 Study of the time step size for the model that partly neglects the time history of the fine scales. (a) Mean stream-wise velocity. RMS velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 5.11 Study of the time step size for the model that accounts for the time dependence of the fine scales. (a) Mean stream-wise velocity. RMS velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 5.12 Planview of the airfoil problem

Figure 5.13 Detail of the tetrahedral mesh around the airfoil
Figure 5.14 (a) Velocity streamlines and q-criterion iso-surfaces (b) Detail of the streamlines on the upper side of the airfoil. This figure has been generated by Mark Vanmoer of the National Center for Supercomputing Applications.
Figure 5.15 Mean velocity and streamlines at Re = 60,000 employing the finest tet-10 mesh

Figure 5.16 Mean pressure coefficient on the surface of the airfoil

Figure 5.17 Mean drag coefficient on the surface of the airfoil
Box 5.1 Algorithmic form of the model

1. Initialize the algorithm: \( i = 1, \ n = 1, \ t = 0, \ v_i^0 = v_0, \ \frac{\partial v_i}{\partial t} \bigg|_0 = 0, \ p_i^0 = 0 \).

2. Update time level, \( t \leftarrow t + \Delta t \) and the time step counter, \( n \leftarrow n + 1 \).

3. Compute the predictor variables: \( v_i^n = v_i^{n-1}, \ p_i^n = p_i^{n-1} \) and \( \frac{\partial v_i}{\partial t} \bigg|_n = \gamma - 1 \frac{\partial v_i}{\partial t} \bigg|_0 \), and reset the iteration counter, \( i = 1 \).

4. Compute the stabilization tensor \( \boldsymbol{\tau}_{\mu} \) for the stabilization of fine-scale level-I using eq. (5.35).

5. Compute the fine-scales level-I \( v' \) and \( p' \) using eq. (5.41).

6. Employing eq. (5.48), compute the element consistent tangent matrices \( (\mathbf{K}^{e})_i^n \) and element residual vectors \( (\mathbf{R}^{e})_i^n \) and assemble them to form the linearized system

\[
\mathbf{K}_i^n \Delta \mathbf{d}_i = \mathbf{R}_i^n, \text{ where } \Delta \mathbf{d}_i = \left[ \Delta v_i^n, \Delta p_i^n \right]^T.
\]

7. Apply the Dirichlet boundary conditions to the linear system of equations formed in step 6.

8. Solve the linear system formed in steps 6 and 7.

9. Update the solution vectors: \( \left[ v_{i+1}^n, p_{i+1}^n \right]^T = \left[ v_i^n, p_i^n \right]^T + \left[ \Delta v_i^n, \Delta p_i^n \right]^T \) and

\[
\frac{\partial v}{\partial t} \bigg|_{i+1} = \frac{\partial v}{\partial t} \bigg|_i + \frac{1}{\gamma \Delta t} \Delta v_i^n.
\]

10. If convergence criterion is not satisfied, update the nonlinear iteration counter, \( i \leftarrow i + 1 \), and go to step 4. Else, continue with step 11.

11. Update the converged solution: \( v^n = v_{i+1}^n, \ p^n = p_{i+1}^n \) and \( \frac{\partial v}{\partial t} \bigg|_{i+1} = \frac{\partial v}{\partial t} \bigg|_i \).

12. If \( n \) is the last time step stop, else go to step 2.
Table 5.1 Location of the separation and reattachment of the boundary layer Re = 60,000

<table>
<thead>
<tr>
<th></th>
<th>Separation</th>
<th>Reattachment</th>
<th>Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental [107]</td>
<td>0.30</td>
<td>0.62</td>
<td>0.32</td>
</tr>
<tr>
<td>Numerical [42]</td>
<td>0.23</td>
<td>0.65</td>
<td>0.42</td>
</tr>
<tr>
<td>Numerical [130]</td>
<td>0.2069</td>
<td>0.6658</td>
<td>0.4589</td>
</tr>
<tr>
<td>Mesh 1, $\Delta t = 0.005$ (Tet-10)</td>
<td>0.2127</td>
<td>0.6867</td>
<td>0.4740</td>
</tr>
<tr>
<td>Mesh 2, $\Delta t = 0.005$ (Tet-10)</td>
<td>0.2093</td>
<td>0.6947</td>
<td>0.4854</td>
</tr>
<tr>
<td>Mesh 2, $\Delta t = 0.0025$ (Tet-10)</td>
<td>0.2229</td>
<td>0.6865</td>
<td>0.4636</td>
</tr>
<tr>
<td>Mesh 3, $\Delta t = 0.005$ (Hex-8, [98] formulation)</td>
<td>0.2333</td>
<td>0.6768</td>
<td>0.4435</td>
</tr>
</tbody>
</table>
Chapter 6

A three-scale residual-based turbulence model for problems with moving boundaries

6.1 Motivation

This Chapter presents a turbulence model for incompressible flows in domains with moving boundaries. The method is an extension of our previous work on turbulence models for problems with fix boundaries [98, 21]. The formulation is derived employing the Variational Multiscale (VMS) framework, which was introduced by Hughes and co-workers [64, 65], and was later extended to turbulence modeling, see e.g. [66, 26, 106, 47, 35, 2, 25, 43, 49, 98, 21] and references therein. To accommodate problems with moving boundaries, the formulation is cast in an Arbitrary Lagrangian-Eulerian (ALE) frame of reference.

In the VMS framework, the solution fields are decomposed in overlapping components of different scales. The largest scales, termed the coarse scales, are represented by the finite element discretization, while the smallest scales, termed the fine scales, are modeled in terms of the coarse-scale fields. If the multiscale decomposition is applied to both the velocity and pressure fields, the problem that governs the fine scales is a mixed-field problem. In [21], we VMS-stabilized the fine-scale problem by further decomposing the fine-scales in two other hierarchical scales termed level-I and level-II fine scales. The model for the level-II scales is variationally embedded in the problem that governs the level-I scales with the goal of enhancing its stability. The model for the level-I scales is employed to model the effects of the sub-grid fields on the coarse-scale problem and stabilize the coarse-scale formulation. To derive the models for the level-I and level-II scales, we use a bubble functions approach that enables the derivation of models that do not have any embedded or tunable parameters. Similar bubble function approaches have also been successfully applied by Masud and co-workers to model several fluid mechanics problems [92, 96, 97]. Turbulence models that are VMS-based have common roots with traditional LES models [9, 29, 102, 122]. In the two approaches, the largest features of the flow are numerically resolved,
while the effects of the sub-grid scales are accounted for via some modeling terms that are present in the formulation that governs the resolvable scales.

To model problems with moving boundaries, two main families of approaches have been proposed in the literature. Interface-capturing techniques [27, 135, 31, 82] use a fix mesh to solve the fluid equations. To accommodate the moving boundaries, the solution fields are augmented with a scalar field that tracks the location of the moving boundary. The advantage of this class of methods is that the boundaries can undergo large deformations without the need of re-meshing. On the other hand, in interface-tracking techniques the nodes that are initially on the moving boundaries remain on the moving boundaries, and the other mesh nodes are updated to minimize the mesh distortion. The main class of interface-tracking methods is based on the ALE frame of reference [57, 77, 117, 12, 20]. The advantage of ALE techniques is that, in most of the cases, the elements located in boundary layers that are adjacent to a moving boundary move with the boundary. Therefore the mesh length-scale in the boundary layer region is approximately conserved. This fact makes ALE techniques a very powerful framework to study problems in which re-meshing is not needed. In this Chapter we use an ALE frame of reference to accommodate the moving boundaries.

The remaining part of the Chapter is organized as follows. In Sec. 6.2, the incompressible Navier-Stokes equations are presented in an ALE frame. In Sec. 6.3 the three-level multiscale method derived in [21] is extended to problems with moving boundaries. To show the accuracy and applicability of the formulation, in Sec. 6.4 we study the flow around a plunging airfoil. The flow is studied at $Re = 40,000$ and $Re = 60,000$, and the results are compared with experiments and numerical results reported by Visbal et al. [131] for the lowest Reynolds number. Conclusions are presented in Sec. 6.5.

### 6.2 The incompressible Navier-Stokes equations

Let $\Omega_t \subset \mathbb{R}^3$ be an open bounded region with moving piecewise smooth boundary $\Gamma_t = \partial \Omega_t$. The incompressible Navier-Stokes equations, which are defined in the time interval $[0,T]$, can be written in an Eulerian frame of reference as follows:

\[
\left. \frac{\partial \mathbf{v}}{\partial t} \right|_r + \mathbf{v} \cdot \nabla \mathbf{v} - 2\nu \nabla \cdot \mathbf{v} + \nabla p = \mathbf{f} \quad \text{in} \quad \Omega_t \times [0,T] \tag{6.1}
\]
\[ \nabla \cdot \mathbf{v} = 0 \quad \text{in} \quad \Omega \times [0,T] \]  

(6.2)

where \( \mathbf{v} \) is the velocity vector, \( p \) is the kinematic pressure, \( \mathbf{v} \) is the kinematic viscosity which in the present work is assumed to be a positive constant, \( \mathbf{f} \) is the body force vector and \( \varepsilon(\mathbf{v}) = (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)/2 \) is the strain rate tensor. To complement (6.1)-(6.2), boundary and initial conditions are also prescribed:

\[ \mathbf{v} = \mathbf{g} \quad \text{on} \quad \Gamma_{g} \times [0,T] \]  

(6.3)

\[ (2\nu \varepsilon(\mathbf{v}) - p \mathbf{I}) \cdot \mathbf{n}_r = \mathbf{h} \quad \text{on} \quad \Gamma_{h} \times [0,T] \]  

(6.4)

\[ \mathbf{v}(x,0) = \mathbf{v}_0 \quad \text{on} \quad \Omega_0 \times \{0\} \]  

(6.5)

where \( \mathbf{g} \) and \( \mathbf{h} \) are the Dirichlet and Neumann boundary conditions, respectively, \( \mathbf{v}_0 \) is the initial velocity condition, \( \mathbf{n}_r \) is the exterior normal to the moving boundary \( \Gamma \), and \( \mathbf{I} \) is the identity tensor. The Dirichlet and Neumann parts of the boundary, which are denoted as \( \Gamma_{g} \) and \( \Gamma_{h} \), respectively, satisfy the following conditions: \( \Gamma_{g} \cup \Gamma_{h} = \Gamma \) and \( \Gamma_{g} \cap \Gamma_{h} = \emptyset \).

To accommodate the moving boundaries, we cast the problem (6.1)-(6.2) to an ALE frame of reference using the following expression that relates the time derivative of the velocity field in the Eulerian frame of reference \( \frac{\partial \mathbf{v}}{\partial t} \) with the time derivative of the same field in the ALE frame of reference \( \frac{\partial \mathbf{v}}{\partial t} \):

\[ \frac{\partial \mathbf{v}}{\partial t} \bigg|_{\xi} = \frac{\partial \mathbf{v}}{\partial t} \bigg|_{\nu} - \mathbf{v}^{\nu} \cdot \nabla \mathbf{v} \]  

(6.6)

where \( \mathbf{v}^{\nu} \) is the velocity of the mapping between the Eulerian and ALE frames. Substituting (6.6) in (6.1), we obtain the momentum expression in the ALE frame of reference:

\[ \frac{\partial \mathbf{v}}{\partial t} \bigg|_{\nu} + (\mathbf{v} - \mathbf{v}^{\nu}) \cdot \nabla \mathbf{v} - 2\nu \nabla \cdot \varepsilon(\mathbf{v}) + \nabla p = \mathbf{f} \]  

(6.7)

Let \( \mathbf{w}(x) \in \mathcal{V} = \left( H_0^1(\Omega) \right)^3 \) and \( q(x) \in \mathcal{Q} = C^0(\Omega) \cap L^2(\Omega) \) be the weighting functions for the velocity and the pressure fields, respectively. Let \( \mathcal{S} \) and \( \mathcal{P} \) be the time-dependent
space of trial solutions for the velocity and pressure fields, respectively. The standard weak form of problem (6.2)-(6.7) is: Find $\mathbf{v}(\mathbf{x},t) \in \mathcal{S}$ and $p(\mathbf{x},t) \in \mathcal{P}$ such that for all $\mathbf{w}(\mathbf{x}) \in \mathcal{V}$ and $q(\mathbf{x}) \in \mathcal{Q}$:

\[
(w, \frac{\partial \mathbf{v}}{\partial t}) + (w, (\mathbf{v} - v_M) \cdot \nabla \mathbf{v}) + (\nabla' \mathbf{w}, 2\nabla' \mathbf{v}) - (\nabla \cdot \mathbf{w}, p) = (w, f) \tag{6.8}
\]

\[
(q, \nabla \cdot \mathbf{v}) = 0 \tag{6.9}
\]

where $(\cdot, \cdot) = \int_{\Omega} (\cdot) d\Omega$ is the $L^2(\Omega)$-inner product. In (6.8), the time derivative is expressed in the ALE frame of reference, but to keep the formulation simple the sub-index $Y$ has been suppressed.

**Remark:** The system of equations (6.8)-(6.9) constitute the problem for which we develop the Multiscale Variational formulation in Sec. 6.3.

### 6.3 A residual-based turbulence model for problems with moving boundaries

The objective of this section is to develop a formulation that accounts for all the scales involved in the problem (6.8)-(6.9). We follow the same approach that we employed for the case of problems with fix boundaries [21]. However, in the present Chapter, all the derivations are done in an ALE frame of reference to extend the formulation to problems with moving boundaries. To this end, we use the Variational Multiscale framework [64, 95] which assumes a multiscale decomposition of the pressure and velocity fields in coarse scales, denoted as $\overline{(*)}$, and fine scales, denoted as $'(*)$:

\[
\mathbf{v}(\mathbf{x},t) = \overline{\mathbf{v}}(\mathbf{x},t) + v'(\mathbf{x},t) \tag{6.10}
\]

\[
p(\mathbf{x},t) = \overline{p}(\mathbf{x},t) + p'(\mathbf{x},t) \tag{6.11}
\]

In the present work, the coarse scales are represented by the standard finite element shape functions, while the fine scales, which are the part of the solution that cannot be captured by the coarse scales, can be represented by any other interpolation function. The
only requirement on the interpolation functions for the fine scales is that they must be linearly independent of the shape functions employed to represent the coarse scales.

Similarly to the decomposition (6.10)-(6.11), we also assume a multiscale decomposition of the weighting functions \( w(x) \) and \( q(x) \) in components of different scales:

\[
w(x) = \bar{w}(x) + w'(x) \quad (6.12)
\]

\[
q(x) = \bar{q}(x) + q'(x) \quad (6.13)
\]

Although the incompressible Navier-Stokes equations are nonlinear, the variational problem (6.8)-(6.9) is linear with respect to the weighting functions. Thus, substituting (6.10)-(6.13) in (6.8)-(6.9), the variational problem can be decomposed in two coupled subproblems:

**Coarse-scale sub-problem:**

\[
\left( \frac{\partial (\bar{v} + v')}{\partial t} \right)^c + \left( \bar{w}, (\bar{v} + v' - \nu_s) \cdot \nabla (\bar{v} + v') \right)^c + (\nabla' \bar{w}, 2 \nu \nabla' (\bar{v} + v')) - (\nabla \cdot \bar{w}, \bar{p} + p') - (\bar{w}, f) = 0
\]

\[
(q, \nabla \cdot (\bar{v} + v')) = 0 \quad (6.14)
\]

**Fine-scale sub-problem:**

\[
\left( \frac{\partial (\bar{v} + v')}{\partial t} \right)^f + \left( w', (\bar{v} + v' - \nu_s) \cdot \nabla (\bar{v} + v') \right)^f + (\nabla' w', 2 \nu \nabla' (\bar{v} + v')) - (\nabla \cdot w', \bar{p} + p') - (w', f) = 0
\]

\[
(q', \nabla \cdot (\bar{v} + v')) = 0 \quad (6.15)
\]

The coarse and fine-scale sub-problems are transient, nonlinear and coupled. The objective in the VMS framework is to extract a model from (6.16)-(6.17) for the fine-scale fields in terms of the coarse-scales variables, and then variationally project the model to the coarse-scale problem (6.14)-(6.15). Although this procedure results in a formulation that only depends on the coarse-scale variables, the effects of the fine scales are accounted for via the modeling terms projected to the coarse-scale problem.
6.3.1 Modeling of the fine-scale fields

Let us consider the fine-scale problem (6.16)-(6.17). If the terms that do not contain any fine-scale field are moved to the right hand side of the equation, and the viscous and the pressure terms of the coarse scales are integrated by parts to eliminate the derivative operator of their weighting slots, the fine scale problem can be written in the following form:

\[
(w', \frac{\partial v'}{\partial t}) + (w', v' \cdot \nabla \bar{v}) + (w', (\bar{v} - v_M) \cdot \nabla v') \\
+ (w', v' \cdot \nabla v') + (\nabla' w', 2 \nu \nabla' v') - (\nabla \cdot w', p') = -(w', r_M)
\]

(6.18)

\[
(q, \nabla \cdot v') = - (\bar{q}, r_C)
\]

(6.19)

where

\[
r_M = \frac{\partial \bar{v}}{\partial t} + (\bar{v} - v_M) \cdot \nabla \bar{v} - 2 \nu \Delta \bar{v} + \nabla \bar{p} - f
\]

(6.20)

is the residual of the momentum equation of the coarse scales, and

\[
r_C = \nabla \cdot \bar{v}
\]

(6.21)

is the residual of the coarse scale continuity equation.

**Remark:** The variational problem (6.18)-(6.19) that models the fine-scale fields \( v' \) and \( p' \) is a convection-dominated mixed-field problem. Thus, the problem has to be stabilized if arbitrary interpolation functions are to be employed for.

To derive a stabilized formulation for (6.18)-(6.19), we also use the VMS ideas by further decomposing the fine-scale velocity field in two other components termed as level-I scale and level-II scale:

\[
v'(x, t) = v_1'(x, t) + v_{II}'(x, t)
\]

(6.22)

The space of functions employed to represent level-I and level-II scales must be linearly independent. We do not assume a multiscale decomposition for the fine-scale pressure field. If it was assumed, then we would end up with another mixed-field problem to model at level-II scales. Thus,

\[
p'(x, t) = p_1'(x, t)
\]

(6.23)
In the VMS framework, the same decomposition assumed for the solution field is also assumed for the weighting functions. Therefore, we decompose the weighing function of the fine-scale velocity $w'$ in level-I scale $w'_I$ and level-II scale $w'_II$:

$$w'(x) = w'_I(x) + w''_I(x)$$  \hspace{1cm} (6.24)

and we do not further decompose the weighting function of the fine-scale pressure field:

$$q'(x) = q'_I(x)$$  \hspace{1cm} (6.25)

**Remark:** In the present three-level approach, the coarse-scales represent the resolvable features of the flow field. The level-I scales are employed as a turbulence model. In addition, they also provide stability to the coarse-scale problem. The level-II scales are just needed to add VMS-stabilization to the problem that governs the level-I scales.

Substituting (6.22)-(6.25) in (6.18)-(6.19), the fine-scale problem can be decomposed in a variational problem that governs the level-I scales, termed as the fine-scale level-I problem, and a problem that governs the level-II scales, termed as the fine-scale level-II problem:

**Fine-scale problem level-I:**

$$\begin{align*}
(w'_I, \frac{\partial (v'_I + v''_I)}{\partial t}) + (w'_I, (v'_I + v''_I) \cdot \nabla \bar{\nu}) + (w'_I, (\bar{\nu} - v_M) \cdot \nabla (v'_I + v''_I)) \\
+ (\nabla^* w'_I, 2v \nabla' (v'_I + v''_I)) - (\nabla \cdot w'_I, p'_I) = - (w'_I, r_M)
\end{align*}$$  \hspace{1cm} (6.26)

$$(\bar{q}, \nabla \cdot (v'_I + v''_I)) = - (\bar{q}, r_C)$$  \hspace{1cm} (6.27)

**Fine-scale problem level-II:**

$$\begin{align*}
(w''_I, \frac{\partial (v'_I + v''_I)}{\partial t}) + (w''_I, (v'_I + v''_I) \cdot \nabla \bar{\nu}) + (w''_I, (\bar{\nu} - v_M) \cdot \nabla (v'_I + v''_I)) \\
+ (\nabla^* w''_I, 2v \nabla' (v'_I + v''_I)) - (\nabla \cdot w''_I, p'_I) = - (w''_I, r_M)
\end{align*}$$  \hspace{1cm} (6.28)

To solve the coupled problems I and II, we first model the level-II velocity field $v''_I$ in terms of the coarse scales and the level-II scales using (6.28). The model is then variationally embedded in the fine-scale problem level-I (6.26)-(6.27). We assume that the level-II fields
are zero on the element boundaries with the objective of localizing the problem and deriving a computationally economic model:

\[ \mathbf{v}'_H = \mathbf{w}'_H = \mathbf{0} \text{ on } \Gamma' \]  

(6.29)

A class of functions that satisfy the previous condition are bubble functions such as polynomial functions. If \( b^e_H \) is the bubble function employed to represent the level-II scales, the level-II fields can be expressed as:

\[ \mathbf{v}'_H = \mathbf{\beta}_H b^e_H \]  

(6.30)

\[ \mathbf{w}'_H = \mathbf{\gamma}_H b^e_H \]  

(6.31)

where \( \mathbf{\beta}_H \) and \( \mathbf{\gamma}_H \) are the element three-dimensional variables that represent the amplitude of the corresponding fields.

Substituting the interpolations (6.30)-(6.31) in the variational problem (6.28), the level-II velocity field can be approximated as:

\[ \mathbf{v}_H = -\tau_H \left( \mathbf{r}_M + \mathbf{v}'_I \cdot \nabla \mathbf{v} + \left( \mathbf{\bar{v}} - \mathbf{v}_M \right) \cdot \nabla \mathbf{v}'_I - 2 \nu \Delta \mathbf{v}'_I + \nabla p'_I \right) \]  

(6.32)

where the second order tensor \( \tau_H \) is defined as:

\[ \tau_H = b^e_H \left[ \frac{\alpha_m}{\gamma \Delta t} \int \left( b^e_H \right)^2 d\Omega + \alpha_f \hat{\tau} \right]^{-1} \]  

(6.33)

and

\[ \hat{\tau} = \int \left( b^e_H \right)^2 \nabla^T \mathbf{v} d\Omega \]

\[ + \int b^e_H \left( \mathbf{\bar{v}} - \mathbf{v}_M \right) \cdot \nabla b^e_H d\Omega \mathbf{I} + \nu \int \left\| \nabla b^e_H \right\|^2 d\Omega \mathbf{I} + \nu \int \nabla b^e_H \otimes \nabla b^e_H d\Omega \]  

(6.34)

The model of the fine-scale level-II velocity is variationally injected in the level-I problem (6.26)-(6.27), which after reordering the terms, can be written as follows:
\[
\begin{align*}
(w'_{t}, \frac{\partial v'_{t}}{\partial t}) + (w'_{t}, v'_{t} \cdot \nabla v) + (w'_{t}, (\bar{v} - v_{M}) \cdot \nabla v'_{t}) + (\nabla' w'_{t}, 2\nu \nabla' v'_{t}) \\
- (\nabla \cdot w'_{t}, p'_{t}) + (q'_{t}, \nabla \cdot v'_{t}) \\
- (w'_{t} \cdot \nabla^{T} \bar{v} - (\bar{v} - v_{M}) \cdot \nabla w'_{t} - \nabla \cdot (\bar{v} - v_{M}) w'_{t} - 2\nu \Delta \nu w'_{t} - \nabla q'_{t}, \\
\tau_{l} (v'_{t} \cdot \nabla \bar{v} + (\bar{v} - v_{M}) \cdot \nabla v'_{t} - 2\nu \Delta v'_{t} + \nabla p'_{t})) \\
= - (w'_{t}, r_{M}) - (q'_{t}, r_{c}) \\
+ (w'_{t} \cdot \nabla^{T} \bar{v} - (\bar{v} - v_{M}) \cdot \nabla w'_{t} - \nabla \cdot (\bar{v} - v_{M}) w'_{t} - 2\nu \Delta w'_{t} - \nabla q'_{t}, \tau_{ll} r_{M})
\end{align*}
\]

**Remark:** The mixed-field variational problem (6.35) is a VMS-stabilized problem. Therefore, arbitrary interpolation spaces for the level-I velocity and pressure fields can be employed.

The next step is to solve (6.35) to get a model that will be used to account for the fine-scale fields in the coarse-scale problem. Since we have assumed that the fine-scales and the level-II scales are zero on the element boundaries, the level-I scales are also assumed to be zero on the element boundaries to keep the fine-scale problem local:

\[
v'_{t} = w'_{t} = 0 \text{ on } \Gamma'
\]
\[
p'_{t} = q'_{t} = 0 \text{ on } \Gamma'
\]

As it was done in the case of the level-II fields, the level-I fields are expressed in terms of a bubble function \(b_{l}^{c}\):

\[
\begin{pmatrix}
v'_{t} \\
p'_{t}
\end{pmatrix} = \beta_{l} b_{l}^{c} \quad \text{(6.38)}
\]
\[
\begin{pmatrix}
w'_{t} \\
q'_{t}
\end{pmatrix} = \gamma_{l} b_{l}^{c} \quad \text{(6.39)}
\]

where in this case, \(\beta_{l}\) and \(\gamma_{l}\) are four dimensional element quantities used to represent the level-I fields.

**Remark:** Bubble functions \(b_{c}^{l}\) and \(b_{ll}^{c}\) must be linearly independent to achieve a unique decomposition of the fine scales in level-I and level-II. In addition, to have a unique decomposition of the solution fields in coarse and fine scales, their functional spaces must also be linearly independent. For the numerical tests section, linear independence is achieved.
by using quadratic and fourth order polynomial bubbles to represent the level-I and level-II scales, respectively. The coarse scales are represented by standard shape functions.

Substituting (6.38)-(6.39) in the variational problem (6.35), the solution of the fine scale can be expressed in the following form:

\[ \begin{bmatrix} v'_{I} \\ p'_{I} \end{bmatrix} = - b_i^c \tau \begin{bmatrix} r_M \\ r_C \end{bmatrix}_{n+1} + \mathcal{F}(v'_I, p'_I) \]

\[ \text{(6.40)} \]

where \( \tau \) is a second order tensor and \( \mathcal{F} \) is a function that depends on the time history of the level-I scales. Since the level-II scales are only used to stabilize the level-I problem, the fine-scale solution can be approximated by the level-I scales:

\[ \begin{bmatrix} v' \\ p' \end{bmatrix} \approx \begin{bmatrix} v'_{I} \\ p'_{I} \end{bmatrix} \]

\[ \text{(6.41)} \]

**Remark:** The detailed algorithm to compute the second order tensor \( \tau \) and \( \mathcal{F} \) is given in [21] for the case of problems with fix boundaries. In the context of problems with moving boundaries, the coarse-scale advection velocity needs to be substituted by the corrected velocity that accounts for the deformation of the mesh \( \bar{v} - v_M \).

**Remark:** The time history term \( \mathcal{F} \) in (6.40) can be dropped in order to obtain a more economical turbulence model. For the case of problems with fix boundaries, we showed via numerical tests that dropping \( \mathcal{F} \) only decreases the accuracy of the turbulence model for very small time step sizes.

### 6.3.2 The final turbulence model

The objective of the present work is to derive a formulation that only depends on the coarse scales, which are represented by the standard finite element shape functions, but incorporates the effects of the fine-scales. Equation (6.40) is a model for the fine-scale fields that only depends on the coarse scales and the time history of the fine-scales if the functional \( \mathcal{F} \) is retained in the formulation. Substituting the model (6.40) in the problem that governs the coarse scales (6.14)-(6.15), the formulation can be written as:
\[
\begin{align*}
\left(\mathbf{w}, \frac{\partial \mathbf{v}}{\partial t}\right) + \left(\mathbf{w}, \left(\mathbf{v} - \mathbf{v}_M\right) \cdot \nabla \mathbf{v}\right) + \left(\nabla' \mathbf{w}, 2\nu \nabla' \mathbf{v}\right) - \left(\nabla \cdot \mathbf{w}, p\right) + (q, \nabla \cdot \mathbf{v}) \\
+ \left(\mathbf{w}, \frac{\partial \mathbf{v}'}{\partial t}\right) - \left(\left(\mathbf{v} - \mathbf{v}_M\right) \cdot \nabla \mathbf{w} - \nabla \cdot \mathbf{v}_M - \mathbf{w} \cdot \nabla' \mathbf{v} + \nabla q + 2\nu \Delta' \mathbf{w}, \mathbf{v}'\right)
\end{align*}
\] (6.42)

To obtain (6.42) we have combined the weak form of the momentum and continuity equations, we have integrated by parts the terms that contain spatial derivatives of the fine-scale velocity \(v'\), and we have applied the assumption that the fine scales vanish on the elements boundaries. In (6.42), several terms can be identified. The terms of the first line are the terms of the left hand side of the standard variational form (6.8)-(6.9):

\[
B_{\text{Gal}}\left(\mathbf{w}, \mathbf{q} ; \mathbf{v}, p, \mathbf{v}_M\right) = \left(\mathbf{w}, \frac{\partial \mathbf{v}}{\partial t}\right) + \left(\mathbf{w}, \left(\mathbf{v} - \mathbf{v}_M\right) \cdot \nabla \mathbf{v}\right) + \left(\nabla' \mathbf{w}, 2\nu \nabla' \mathbf{v}\right)
\]

\[
- \left(\nabla \cdot \mathbf{w}, p\right) + (q, \nabla \cdot \mathbf{v})
\] (6.43)

and the term on the right hand side is the standard forcing term of (6.8):

\[
F_{\text{Gal}}\left(\mathbf{w}\right) = \left(\mathbf{w}, f\right)
\] (6.44)

The second line of (6.42) appears due to the assumption of the presence of fine-scale fields, and its terms model the effects of the fine scales in the coarse-scale problem. They can be grouped in the following functional:

\[
B_{\text{VMS}}^{\text{Turb}}\left(\mathbf{w}, \mathbf{q} ; \mathbf{v}', \mathbf{p}', \mathbf{v}_M\right) = \left(\mathbf{w}, \frac{\partial \mathbf{v}'}{\partial t}\right) - \left(\left(\mathbf{v} - \mathbf{v}_M\right) \cdot \nabla \mathbf{w} - \nabla \mathbf{v}_M \cdot \mathbf{v}_M
\]

\[
- \mathbf{w} \cdot \mathbf{v}' + \nabla q + 2\nu \Delta' \mathbf{w}, \mathbf{v}'\right)
\] (6.45)

Therefore, we can write the final formulation (6.42) in an abstract form as:

\[
B_{\text{Gal}}\left(\mathbf{w}, \mathbf{q} ; \mathbf{v}, p, \mathbf{v}_M\right) + B_{\text{VMS}}^{\text{Turb}}\left(\mathbf{w}, \mathbf{q} ; \mathbf{v}', \mathbf{p}', \mathbf{v}_M\right) = F_{\text{Gal}}\left(\mathbf{w}\right)
\] (6.46)

Remark: The three-scale residual-based turbulence model accounts for the effects of the fine scales via a hierarchical approach that is used to stabilize the mixed field variational problem and model the sub-grid turbulent features of the flow.
Remark: Most of the terms in (6.46) have the same form as the terms present in the formulation derived in [21] for problem with fixed boundaries. In [21], we give a detailed explanation of how to implement the terms and how to evaluate the fine scale fields.

6.3.3 Mesh moving scheme

The formulation presented in the previous section can accommodate problems with moving boundaries. However, to actually solve this class of problems, the formulation has to be complemented with a technique to move the computational mesh so that it can be adapted to the evolving boundaries of the problem. The displacement of the mesh nodes is usually determined by solving a simple partial differential equation [127]. In the present work we use the technique developed by Masud and co-workers [86, 94, 75].

Let $\Gamma^f$ be the part of the boundary that is fixed, and let $\Gamma^m$ be the part of the boundary that can move. On the moving boundary, the displacement is prescribed using the function $g(x,t)$. The displacement $d(x,t)$ of the mesh is obtained by solving the following modified Laplace problem:

$$
\nabla \cdot \left( [1 + \alpha^e] \nabla d \right) = 0 \quad \text{in } \Omega,
$$

$$
d = g(x,t) \quad \text{on } \Gamma^m,
$$

$$
d = 0 \quad \text{on } \Gamma^f
$$

where $\alpha^e$ is a parameter that depends on the volume $V_e$ of element $e$, the volume of the smallest element of the mesh $V_{\min}$, and the volume of the largest element of the mesh $V_{\max}$:

$$
\alpha^e = \frac{1 - V_{\min}/V_{\max}}{V_e/V_{\max}}
$$

The goal of introducing the parameter $\alpha^e$ is to make the mesh moving technique robust. Its definition makes smaller elements stiffer than larger elements. As a consequence, large elements absorb most part of the deformation of the mesh.

The parameter $\alpha^e$ can be computed using the element volumes of the initial undeformed mesh, or it can be computed at every time step. If the first approach is adopted, the linear system of equations that needs to be solved to move the mesh can be factorized during
the computation of the first time step. For the other time steps, the mesh can be easily updated by just doing backward and forward substitutions. If the value of \( \alpha' \) is recomputed every few time step, the mesh moving scheme is more robust as the elements that become smaller during the evolution of the problem also become stiffer. However, the linear system of equations for the modified Laplace problem needs to be formed and solved every time that \( \alpha' \) is updated. In all the cases, the computational cost of solving the modified Laplace problem is much smaller than the computational cost of solving the Navier-Stokes equations.

### 6.4 Numerical results

To show the applicability and accuracy of the presented method, in this section we study the flow around a plunging airfoil. The flow is studied at \( Re = 40,000 \) and \( Re = 60,000 \). For the lowest Reynolds number flow, the results are compared with experimental and numerical results reported by Visbal and co-workers [131]. The comparison shows the accuracy of the present formulation. For the first studied flow, we also report an extensive set of velocity and pressure profiles that complement the previously published results [131]. The problem is also studied at a higher Reynolds number to show the robustness of the method. In this second case, we also report an extensive set of velocities and pressure profiles along several sections of the computational domain. To assure the accuracy of our results, we have performed the computations employing two meshes and two time step sizes.

We study a prismatic airfoil SD7003 of unit chord \( c \) and with an angle of attack of \( 4^\circ \). The prescribed vertical motion of the airfoil is sinusoidal, i.e., \( y_A = A \sin(kt) \), where the amplitude \( A \) is set equal to 0.05 and the reduced frequency \( k \) is set equal to 3.93. The computational domain employed in the computations is schematically represented in Fig. 6.1. The inflow boundary is a semicircle of radius \( 6c \) and its center is located at the initial center of the airfoil. The lateral boundaries are located at a distance \( 6c \) of the initial location of the airfoil, and the outflow boundary is at \( 6c \) downstream of the airfoil. The thickness of the domain is \( 0.2c \), which is the same as the one used in [131]. A unit longitudinal velocity \( U_\infty \) is prescribed on the inflow boundary, no penetration is imposed the lateral boundaries, and free traction is prescribed on the outflow boundary. There is no need to prescribe a condition for the pressure field because the free traction condition automatically determines the value of its
rigid mode constant. The viscosity of the fluid is set equal to $2.5 \times 10^{-5}$ and $1.66667 \times 10^{-5}$. Thus, the Reynolds number based on the inflow velocity and the airfoil chord is 40,000 and 60,000, respectively.

The computational domain is discretized employing two hexahedral meshes. The meshes are generated extruding 2D quadrilateral meshes. The smaller elements of each mesh are located in the proximity of the airfoil to capture the boundary layers and the features of the flow that interact with the airfoil. The mesh is graded so that the outer region, where the flow is laminar, the elements are larger. The coarsest mesh, which is partially shown in Fig. 6.2, consists of 24 planes of nodes with 69,858 nodes per plane. The total number of nodes and elements is 1,676,592 and 1,600,225, respectively. The second mesh employed in the numerical studies is obtained from a refinement of the elements of the first mesh. This mesh consists of a total of 3,483,360 nodes and 3,327,939 hexahedral elements. To discretize the formulation in time we use the generalized-alpha method [70], and its parameter $\rho_\infty$ is set equal to 0. The time step sizes employed are $\Delta t = 0.00125$ and $\Delta t = 0.00075$. For the coarsest mesh, the flows are studied using the two time step sizes to show that the largest time step is able to resolve all the temporal time scales of the flow. For the finest mesh, only the smallest time step size is employed. The fine scales of the formulation are solved using polynomial bubble functions of second and fourth order for level-I and level-II scales, respectively. Gaussian quadrature rule is employed to evaluate the element level integrals.

In all the cases, the flow is initialized at $t = 0$ from rest and the inflow boundary condition is increased at a constant rate until it reaches its maximum magnitude at $t = 6.395$. During this time interval, the magnitude of the plunging displacement of the airfoil $A$ also increases linearly from 0 to its maximum value. Then the flow is let to evolve until $t = 15$ when it is statistically periodic. The solution is sampled every 5 time steps in the next 10 units of time.

Figure 6.3 shows iso-surfaces of the instantaneous vorticity field at $Re = 40,000$. The flow is laminar upstream of the airfoil. The boundary layer on the upper side of the airfoil detaches and generates vortices that become fully turbulent after a transitional regime. On the lower side of the airfoil the boundary also detaches, but in this case, the generated vortices remain laminar until they interact downstream of the airfoil with the turbulent vortices.
generated on the upper side. The mean vorticity field can be observed in Fig. 6.4. The four sub-figures, which represent four evenly distributed time instants in a cycle of the plunging movement, show how the vortices are generated and convected downstream.

There are two main differences between the flow around the plunging airfoil studied here and an equivalent fix airfoil [42, 130, 21]. On the lower side of the fix airfoil, the flow is completely laminar and the boundary layer never detaches, while here the flow is much more involved. The other main difference is on the boundary layer of the upper side. The detachment and transition to turbulence happens closer to the trailing edge for the case of the fix airfoil. Looking at the upper side, the plunging movement has the effect of increasing the effective angle of attack.

The evolution of the mean drag and lift coefficients over time is represented in Fig. 6.5. The figure shows the results obtained with the coarsest mesh using time step sizes $\Delta t = 0.00125$ and $\Delta t = 0.00075$, the results of the finest mesh employing $\Delta t = 0.00075$, and numerical results reported by Visbal et al. [131] with $\Delta t U_{\infty}/c = 0.00005$. Despite the time step sizes that we use are two orders of magnitude larger than [131], all our numerical tests agree well with the previously published results. In addition, the mesh and time step size refinement study performed also shows that the results obtained with the present method are converged.

Figures 6.6-6.8 show the mean stream-wise velocity profile along three transversal sections located at $x = 1$, $x = 1.25$ and $x = 1.5$, respectively. For each of the figures, sub-figure (a) shows the mean solution at phase $\phi = 0$, when the airfoil is at $y_A = 0$ and is moving upwards. Sub-figures (b), (c) and (d), correspond to the phases $\phi = \pi/4$, $\phi = \pi/2$ and $\phi = 3\pi/4$, respectively. Each of the plots shows the results obtained from the three numerical tests performed, and confirm the temporal and spatial convergence of the results. Figure 6.8, in addition to show our results, also shows the results obtained computationally and experimentally by Visbal and co-workers [131]. It can be concluded that, our results agree well with [131].

In a similar manner, Figs. 6.9-6.11 show the mean pressure field along three different transversal sections, and for each of the sections, the mean pressure is represented at four representative phases of plunging movement. Due to the lack of previously reported results,
we only show the results obtained with the present formulation. However, the spatial and temporal convergence studies show that the results are accurate.

The same study is repeated at $Re = 60,000$. The flow is studied employing the same two meshes and the same time step sizes as the ones used for the case of $Re = 40,000$. Figure 6.12 shows the mean drag and lift coefficients for the three numerical tests that we have conducted. As in the previous cases, for the higher Reynolds number flow the chosen mesh resolutions and time step sizes are adequate to capture accurately the flow features. The mean stream-wise velocity field along the lines $x = 1$, $x = 1.25$ and $x = 1.5$ is represented in Figs. 6.13-6.15, respectively, and the mean velocity field is represented along the same sections in Figs. 6.16-6.18, respectively. In all the cases, the results obtained with the two meshes and time step sizes agree well with each other.

### 6.5 Conclusions

We have presented a three-scale turbulence model for problems with moving boundaries. The work is an extension of our earlier work on turbulence models for problems with fixed boundaries [21]. All the derivations have been expressed in an ALE frame of reference to accommodate the moving boundaries. The presented method is based on the Multiscale Variational Method, which assumes a decomposition of the solution fields in coarse and fine-scales. This leads to two coupled mixed-field problems that govern the coarse and fine scales. The key idea of the VMS framework is to solve the fine-scale problem and extract a fine-scale model in terms of the coarse-scale fields. The fine-scale model is variationally projected to the coarse scale problem. This yields a formulation that only depends on the coarse scales, but the effects of the fine-scale scales are accounted for by means of the additional terms that appear due to the multiscale decomposition. In the present work, the mixed-field fine-scale problem has been solved employing a VMS stabilization, which has been derived by further decomposing the fine-scale velocity field in two other components termed as level-I and level-II scales. The level-II scales stabilize the problem that govern the level-I scales, and the level-I scales are used as a turbulence model for the coarse scales. The level-I scales are also used to stabilize the coarse-scale problem. One of the main features of the proposed method is that does not have any embedded or tunable parameters. In
addition, due to the three-level approach, the derived sub-grid models represent well the fine-scale features of the fluid flow, and as a results, the resulting formulation is highly accurate.

To show the accuracy and applicability of the developed formulation, we have studied the flow around a plunging airfoil at $Re = 40,000$ and have compared the results with experimental and numerical results reported by Visbal and co-workers [131]. We have also studied the same airfoil at $Re = 60,000$ to show the robustness of the method for more complex flows. In all the cases, we performed the numerical tests using two different meshes and time step sizes to show that the obtained solutions are the converged solutions.

6.6 Figures

![Figure 6.1 Schematic representation of the computational domain](image-url)
Figure 6.2 Plane view of the coarsest mesh

Figure 6.3 Instantaneous vorticity field at Re = 40,000
Figure 6.4 Mean vorticity at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$.

Re = 40,000
Figure 6.5 Mean (a) drag and (b) lift coefficients. Re = 40,000
Figure 6.6 Mean velocity along the line $x = 1$. at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 40,000
Figure 6.7 Mean velocity along the line $x = 1.25$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 40,000
Figure 6.8 Mean velocity along the line $x = 1.5$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 40,000
Figure 6.9 Mean pressure along the line $x = 1$. at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. $Re = 40,000$
Figure 6.10 Mean pressure along the line \( x = 1.25 \) at (a) \( \phi = 0 \), (b) \( \phi = \pi/4 \), (c) \( \phi = \pi/2 \) and (d) \( \phi = 3\pi/4 \). Re = 40,000
Figure 6.11 Mean pressure along the line $x = 1.5$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. $Re = 40,000$
Figure 6.12 Mean (a) drag and (b) lift coefficients. Re = 60,000
Figure 6.13 Mean velocity along the line $x = 1$. at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 60,000
Figure 6.14 Mean velocity along the line $x = 1.25$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 60,000
Figure 6.15 Mean velocity along the line $x = 1.5$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. $Re = 60,000$
Figure 6.16 Mean pressure along the line $x = 1$. at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 60,000
Figure 6.17 Mean pressure along the line $x = 1.25$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 60,000
Figure 6.18 Mean pressure along the line $x = 1.5$ at (a) $\phi = 0$, (b) $\phi = \pi/4$, (c) $\phi = \pi/2$ and (d) $\phi = 3\pi/4$. Re = 60,000
Chapter 7

A Variational Multiscale method for incompressible turbulent flows with free surfaces

7.1 Motivation

Fluid flows with free surfaces are present in many engineering problems. For example, the design and analysis of off-shore structures such as oil platforms and wind turbine farms are problems in which free surfaces play an important role. An accurate representation of free surfaces is also important to capture the effect of waves on coastal structures. All these applications are gaining attention due to the growing interest in new energy sources, and the need to build structures that are able to resist potential environmental hazards caused by climate change. Another area in which free surface dynamics is important is that of fluid sloshing in tanks. Although, sloshing can be an undesirable effect of fluid transportation, it can also be deliberately designed to have an effect on contiguous structures. For instance, sloshing fluids can be employed as energy sink systems, which may mitigate earthquake effects on built structures. Other problems in which free surfaces are important are fluid flow in rivers and channels, and ship hydrodynamics. In all the cases, an accurate modeling of the free surface is crucial for modeling the overall problem of interest.

Several approaches have been adopted to study free surface flows. Interface-tracking techniques are one of the main families of methods. In these methods, the free surface is defined by a set of nodes or particles with an evolving location that tracks the geometry of the free surface. One of the first classes of methods to be proposed is based on the Arbitrary Lagrangian-Eulerian (ALE) framework [57, 56], in which the ALE frame of reference enables the motion of the boundaries and the nodal coordinates. The main limitation of such methods is that when the free surface undergoes very large deformations, the computational mesh needs to be redefined in order to avoid excessive mesh distortion. Particle methods, which are based on a Lagrangian description of the fluid, such as the Particle Finite Element Method (PFEM) [110, 28], overcome the mesh distortion issues. The Lagrangian description of the
fluid and the fact that a mesh is not needed, make these methods suitable for problems with very large deformations of the free surface. Despite their versatility, particle methods are computationally expensive due to the need of determining a tessellation at each time step. The tessellation is needed to compute the interaction between the particles. The ALE/Lagrangian method [28] is a compromise between the two approaches. The region near the free surfaces is modeled employing a particle method that enables the free surface to undergo large deformations, and the remaining part of the domain is modeled using an ALE frame. Space-time methods for free surface problems [124, 125] also fall into the category of interface-tracking methods. In these methods, the space-time domain evolves in the time coordinate axes to describe the motion of the moving free surface.

A second family of methods used to study free surface flows is based on interface-capturing techniques. In this approach, the computational mesh is fix and the location of the free surface is traced employing an additional scalar field. One of the first methods to be proposed in this category is the Volume of Fluids (VOF) technique [54, 31, 84, 82], which uses a scalar field that represents the fraction of fluid in the each of the mesh elements. Another technique is the Level Set method [120, 3], in which the additional field introduced to capture the interface represents the distance to the free surface.

In the present Chapter we develop a model for turbulence flows with free surfaces that is based on the Variational Multiscale (VMS) framework. To accommodate free surfaces, the formulation is cast in an ALE frame of reference. The VMS method was proposed by Hughes [64] and was later extended to turbulence modeling [65, 66, 106, 10, 117, 43]. In the VMS framework, the solution fields are decomposed in components of different scale, namely, the coarse scales and the fine scales. The fine scales are modeled in terms of the residual of the Euler-Lagrange equations for the coarse scales, and the models are variationally injected in the coarse-scale equations. Here we extend the formulation that we presented in [100] on turbulence models for domains with moving boundaries. In [100], we presented a model based on a three-scale decomposition of the velocity and pressure fields. The coarse scales are the ones that represent the resolved scales. The fine scales of the problem are further decomposed into two additional scales termed as level-I and level-II scales. The level-I scales serve as a turbulence model and stabilized the coarse-scale problem. The level-II scales stabilize the problem that governs the level-I scales. In our approach, we use linear shape
functions to represent the coarse-scale fields, and bubble functions for the two levels of fine scales. The bubble functions are a convenient way to model the fine scales because they circumvent the need of any tunable parameter. The numerical properties of the method derived using this approach has been shown in a variety of fluid problems involving laminar flows both in fix [97] and moving domains [20], and turbulent flows also in fix [98, 21] and moving domains [100]. In the present Chapter we extend [100] to problems with free surfaces. To show the applicability and accuracy of our method, we study two turbulent free surface problems. Due to the simple set up of the proposed numerical tests, they have the potential of becoming reference problems for validating models for incompressible turbulent flows that have free surfaces.

The remaining part of the Chapter is organized as follows. In Sec. 7.2, the incompressible Navier-Stokes equations are presented in an ALE frame of reference. In the following section, a method for solving turbulent free surface flows is presented. In Sec. 7.4, we apply the developed model for turbulent flows with free surfaces to two open channel problems. First, we study the flow on a flat open channel. The turbulent features of the flow are the driving mechanism that makes the free surface to deform. To study the flow, we consider two different slopes of the channel. A mesh refinement study shows the convergence of the results. The second problem that we present is a channel with an undulated bottom surface. Multiple flow conditions are studied, and the results obtained for one of the settings are compared with experimental [7] and numerical results [136]. Conclusions are drawn in Sec. 7.5.

### 7.2 The incompressible Navier-Stokes equations

Let \( \Omega \subset \mathbb{R}^3 \) be a connected, open, bounded region with time-dependent piecewise smooth boundary \( \Gamma \). The incompressible Navier-Stokes equations written in an Arbitrary Lagrangian-Eulerian (ALE) frame of reference are:

\[
\begin{align*}
\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} - \mathbf{v}^m) \cdot \nabla \mathbf{v} - 2\nu \nabla \cdot \varepsilon(\mathbf{v}) + \nabla p &= \mathbf{f} \\
\nabla \cdot \mathbf{v} &= 0 \quad \text{in} \; \Omega \times ]0,T[ 
\end{align*}
\]
\[ v = g \quad \text{on} \quad \Gamma_s \big|_t \times ]0,T[ \] 

(7.3)

\[ (2\varepsilon(v) - pI) \cdot n_t = h \quad \text{on} \quad \Gamma_n \big|_t \times ]0,T[ \] 

(7.4)

\[ (2\varepsilon(v) - pI) \cdot n_t = 0 \quad \text{on} \quad \Gamma_j \big|_t \times ]0,T[ \] 

(7.5)

\[ (v - v^m) \cdot n_t = 0 \quad \text{on} \quad \Gamma_j \big|_t \times ]0,T[ \] 

(7.6)

\[ v(x,0) = v_0 \quad \text{on} \quad \Omega_0 \times \{0\} \] 

(7.7)

where \( v \) is the velocity vector, \( p \) is the kinematic pressure, \( f \) is the body force, the positive constant \( \nu \) is the kinematic viscosity, \( v^m \) is mesh velocity, \( \frac{\partial v}{\partial t} \big|_v \) is the time derivative of the velocity field in the ALE frame of reference, \( I \) is the identity tensor, \( n_t \) is the exterior normal to the boundary \( \Gamma_j \), \( v_0 \) is the initial condition for the velocity field, \( \varepsilon(v) = \nabla'v \) is the strain rate tensor, \( g : \Gamma_s \big|_t \rightarrow \mathbb{R}^3 \) is the Dirichlet boundary condition, and \( h : \Gamma_n \big|_t \rightarrow \mathbb{R}^3 \) is the Neumann boundary condition. Without loss of generality, the surface tension on the free surface of the fluid \( \Gamma_f \big|_t \) is assumed to be negligible, i.e. equation (7.5). Equation (7.6) imposes that the free surface boundary moves to fulfill the condition that the flux of fluid across the free surface is zero.

The standard weak form of the problem (7.1)-(7.7) is: find \( v(x,t) \in \mathbf{S} \) and \( p(x,t) \in \mathbf{P} \) such that for all \( w(x) \in \mathbf{V} \) and \( q(x) \in \mathbf{Q} \),

\[ (w, \frac{\partial v}{\partial t}) + (w, (v - v^m) \cdot \nabla v) + (\nabla'w, 2\nu\nabla'v) - (\nabla \cdot w, p) = (w, f) \] 

(7.8)

\[ (q, \nabla \cdot v) = 0 \] 

(7.9)

where \((\cdot, \cdot) = \int_{\Omega} (\cdot) d\Omega\) is the \( L^2(\Omega) \) -inner product. The functions \( w(x) \in \mathbf{V} = \left( H_o^1(\Omega) \right)^3 \) and \( q(x) \in \mathbf{Q} = C^0(\Omega) \bigcap L^2(\Omega) \) are the weighting functions for the velocity and the pressure fields, respectively, and \( \mathbf{S} \) and \( \mathbf{P} \) be the time-dependent space of trial solutions for the velocity and pressure fields, respectively.

The variational problem can also be expressed in a more compact form as:
\[ \mathcal{L}(w; v, p; v_M) = \mathcal{H}(q; v) = 0 \]  

where the functional \( \mathcal{L}(w; v, p; v_M) \) contains all the terms of the left hand side of (7.8), \( \mathcal{H}(q; v) = (q, \nabla \cdot v) \).

### 7.3 The Variational Multiscale method

The variational problem (7.10)-(7.11) is a mixed-field problem, and therefore, it needs to be stabilized in order to employ arbitrary interpolations for the velocity and pressure fields. In addition, the discretization of the domain implicitly filters out some of the scales that are relevant to the problem because they cannot be represented by the chosen discretization. Thus, in order to stabilize the formulation and account for the effects of these flow features that are filtered out, some kind of model needs to be employed. To derive a formulation that addresses the two mentioned issues we use the VMS framework, which decomposes the solution fields in components of different scale. In the next section we briefly present the method that we derived in [100] and then we discuss how to treat the free surface condition considered in the present work.

#### 7.3.1 Multiscale decomposition of the variational problem

The VMS method assumes a multiscale decomposition of the solution fields in components of different scale termed as coarse and fine scales:

\[
\begin{align*}
    v(x, t) &= \bar{v}(x, t) + v'(x, t) \\
    p(x, t) &= \bar{p}(x, t) + p'(x, t)
\end{align*}
\]  

(7.12)  

(7.13)

In order to have a unique decomposition, the functional spaces that define the coarse and fine-scale components must be linearly independent. Similarly, we also decompose the weighting functions \( w \) and \( q \) in coarse and fine scales:

\[
\begin{align*}
    w(x) &= \bar{w}(x) + w'(x) \\
    q(x) &= \bar{q}(x) + q'(x)
\end{align*}
\]  

(7.14)

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\[ q(x) = \overline{q}(x) + q'(x) \]  

Substituting (7.12)-(7.15) to the variational problem (7.10)-(7.11), and employing the fact that the operators \( \mathbf{L} \), \( \varphi \) and \( \mathbf{H} \) are linear with respect to their weighting functions, the problem can be decomposed in two sub-problems:

**Coarse-scale sub-problem:**

\[ \mathcal{L}(\overline{w}; \overline{v} + v', \overline{p} + p'; v_M) = \varphi(\overline{w}) \]  

(7.16)

\[ \mathcal{H}(\overline{q}; \overline{v} + v') = 0 \]  

(7.17)

**Fine-scale sub-problem:**

\[ \mathcal{L}(w'; \overline{v} + v', \overline{p} + p'; v_M) = \varphi(w') \]  

(7.18)

\[ \mathcal{H}(q'; \overline{v} + v') = 0 \]  

(7.19)

In our earlier work on the Navier-Stokes equations [97, 20, 98] we only assumed a multiscale decomposition of the velocity field, and the pressure field was not decomposed. However, the studies that we carried out in [98] we showed that the continuity condition (7.2) is better enforced if the final formulation has a \( \text{div} \)-stabilization term. This term can be derived by assuming a multiscale decomposition of the pressure field in addition to the decomposition of the velocity field. Although the split of the pressure field yield formulations that have superior mass conservation properties, it gives rise to a fine-scale problem that is a mixed-field problem, while the fine-scale problem that corresponds to the first approach is a single field problem.

The procedure employed to solve the coupled coarse and fine-scale problems, is summarized as follows. First, a model for the fine scales \( v' \) and \( p' \) is extracted from fine-scale problem (7.18)-(7.19) in terms of the coarse scales \( \overline{v} \) and \( \overline{p} \). Then, the model is variationally injected into the coarse-scale problem (7.16)-(7.17). Despite the obtained formulation only depends on the coarse scales, the effects of the fine scales are accounted for via the projected fine-scale model.
7.3.2 Solution of the fine-scale problem

The fine-scale problem (7.18)-(7.19) is a mixed field problem, and thus it needs to be stabilized in order to be solved employing arbitrary interpolations for the fine-scale velocity and pressure fields. In a similar approach to the one adopted for the original problem (7.10)-(7.11), we also employ the VMS ideas to derive a stabilized formulation for the fine-scale problem (7.18)-(7.19). Thus, we assume a multiscale decomposition of the velocity field in two components of different scale termed as fine-scale level-I and level-II:

\[ \mathbf{v}'(\mathbf{x},t) = \mathbf{v}'_I(\mathbf{x},t) + \mathbf{v}'_II(\mathbf{x};t) \]  \hspace{1cm} (7.20)

Since the objective of applying the VMS framework to the fine-scale problem is to stabilize the fine-scale problem, which will be used to extract a model that will be employed to account for the sub-grid scales, we do not assume a multiscale decomposition of the fine-scale pressure field:

\[ p'(\mathbf{x},t) = p'_I(\mathbf{x},t) \]  \hspace{1cm} (7.21)

As in the case of the multiscale decomposition applied to (7.18)-(7.19), the level-I and level-II components must be linearly independent in order to have a unique multiscale decomposition. In a similar manner to (7.20)-(7.21), we also decompose the fine-scale component of the weighting velocity field in level-I and level-II components. However, we do not decompose the fine-scale weighing function of the pressure field:

\[ \mathbf{w}'(\mathbf{x}) = \mathbf{w}'_I(\mathbf{x}) + \mathbf{w}'_II(\mathbf{x}) \]  \hspace{1cm} (7.22)

\[ q'(\mathbf{x}) = q'_I(\mathbf{x}) \]  \hspace{1cm} (7.23)

We substitute the decompositions (7.20)-(7.23) to the fine-scale problem (7.18)-(7.19), and exploiting the linearity with respect to the weighting functions \( \mathbf{w}' \) and \( q' \), we can split the fine-scale sub-problems in two other sub-problems as follows:

**Fine-scale problem level-I:**

\[ \mathcal{L}(\mathbf{w}'_I; \overline{\mathbf{v}} + \mathbf{v}'_I + \mathbf{v}'_II; \overline{p} + p'_I; \mathbf{v}_M) = \varphi(\mathbf{w}'_I) \]  \hspace{1cm} (7.24)
\[ \mathcal{H}(q'_i; \bar{v} + v'_i + v''_\text{II}) = 0 \]  

(7.25)

**Fine-scale problem level-I:**

\[ \mathcal{L}(w''_\text{II}; \bar{v} + v'_i + v''_\text{II}, \bar{p} + p'_i; v_M) = \varphi(w''_\text{II}) \]  

(7.26)

**Remark:** The present approach results in an homogeneous multiscale framework because the same operators \( \mathcal{L} \) and \( \mathcal{H} \) govern the three hierarchical problems involved in the decomposition, i.e. problems (7.16)-(7.17), (7.24)-(7.25) and (7.26).

We extract \( v''_\text{II} \) from (7.26) in terms of the coarse scales and level-I scales. To do so, we employ a bubble function to interpolate the level-II velocity field. In the numerical tests section, to solve this problem we use a fourth order polynomial bubble function. This leads to a model that can be expressed in an abstract form as follows:

\[ v''_\text{II} = \mathcal{M}_\text{II}(\bar{v}, \bar{p}, v'_i, p'_i) \]  

(7.27)

We variationally project the model for \( v''_\text{II} \) to the level-I problem (7.24)-(7.25), which can be expressed as:

\[ \mathcal{L}(w'_i; \bar{v} + v'_i + \mathcal{M}_\text{II}(\bar{v}, \bar{p}, v'_i, p'_i, \bar{p} + p'_i; v_M) = \varphi(w'_i) \]  

(7.28)

\[ \mathcal{H}(q'_i; \bar{v} + v'_i + \mathcal{M}_\text{II}(\bar{v}, \bar{p}, v'_i, p'_i)) = 0 \]  

(7.29)

Equations (7.28)-(7.29) only depend on the coarse-scale and level-I fields. Using quadratic bubble functions, which are linearly independent of the fourth order bubbles employed to derive the model (7.27), we can solve (7.28)-(7.29) and derive a model for the level-I scales in terms of the coarse-scale fields:

\[ \begin{bmatrix} v'_i \\ p'_i \end{bmatrix} = \mathcal{M}_\text{I}((\bar{v}, \bar{p})) \]  

(7.30)

Since the level-II scales are just used to stabilize the fine-scale problem (7.18)-(7.19), and the level-I scales are employed to solve the stabilized fine-scale problem (7.28)-(7.29), the fine-scales can be approximated by the level-I solution:

\[ \begin{bmatrix} v' \\ p' \end{bmatrix} \approx \begin{bmatrix} v'_i \\ p'_i \end{bmatrix} \]  

(7.31)
7.3.3 The variational multiscale turbulence model

The model for the fine-scale fields (7.31) is injected to the coarse-scale problem (7.16)-(7.17), which then can be written as follows:

\[ B_{Gal}(\bar{w}, \bar{q} ; \bar{v}, \bar{p}, v_M) + B_{VMS}^{Turb}(\bar{w}, \bar{q} ; \bar{v}, v', p', v_M) = F_{Gal}(\bar{w}) \]  

(7.32)

where

\[ B_{Gal}(\bar{w}, \bar{q} ; \bar{v}, \bar{p}, v_M) = \left( \bar{w}, \frac{\partial \bar{v}}{\partial t} \right) + \left( \bar{w}, (\bar{v} - v_M) \cdot \nabla \bar{v} \right) + \left( \nabla' \bar{w} , 2v \nabla' \bar{v} \right) \]

\[ - (\nabla \cdot \bar{w}, \bar{p}) + (\bar{q}, \nabla \cdot \bar{v}) \]  

(7.33)

is a functional that groups all the terms that appear on the left hand side of the standard variational form (7.8)-(7.9),

\[ F_{Gal}(\bar{w}) = (\bar{w}, f) \]  

(7.34)

is the right hand side of (7.8), and

\[ B_{VMS}^{Turb}(\bar{w}, \bar{q} ; \bar{v}, v', p', v_M) = \left( \bar{w}, \frac{\partial v'}{\partial t} \right) - \left( (\bar{v} - v_M) \cdot \nabla \bar{w} - \bar{w} \nabla \cdot v_M \right) \]

\[ - \bar{w} \cdot \nabla' \bar{v} + \nabla \bar{q} + 2v \Delta' \bar{w} , v' \right) \]

\[ - (\nabla \cdot \bar{w}, v' \otimes v') - (\nabla \cdot \bar{w}, p') \]  

(7.35)

are the terms that arise due to the assumption of the existence of fine scales. The terms of equation (7.35), model the effects of the sub-grid scales on the coarse-scale problem. On the one hand, they provide stability to the mixed field problem, and on the other hand, they also serve as a turbulence model.

Remark: Since the fine-scale fields (7.30) only depend on the coarse scales, the final formulation (7.32) only depends on the coarse-scale fields \( \bar{v} \) and \( \bar{p} \).

7.3.4 Free surface condition

The turbulence model (7.32) is complemented by the condition that enforces a zero fluid flux across the free surface (7.6). Several techniques can be applied to enforce the zero-flux condition. For a detailed discussion see [133]. In the numerical tests section we impose the condition in a weak form, which can be written as follows:
\[
\int_{\Gamma} w(v - v^n) \cdot n_I dI = 0
\]  

(7.36)

where \( w \) is an arbitrary weighting function.

Imposing the zero-flux condition on a weak sense has two main advantages. First, the global mass of the fluid is conserved because the local errors due to the discretization are compensated globally. The second advantage is that the normal \( n_I \) has to be computed only at Gauss points, where the normal is uniquely defined. This is an important advantage with respect to imposing the zero-flux condition weakly, where the normal has to be computed at the nodal points, and is not uniquely defined due to the finite element discretization.

### 7.3.5 Mesh moving scheme

Once the location of the nodes of the free surface has been determined, the location of the other nodes must be updated in order to maintain a good mesh quality. To update the mesh we use the method proposed by Masud and co-workers \([94, 75]\), in which the displacement of the nodal coordinates is determined by the solution of the following modified Laplace problem:

\[
\nabla \cdot \left( \left[ 1 + \alpha^e \right] \nabla d \right) = 0 \quad \text{in } \Omega_e
\]  

(7.37)

\[
d = g(x, t) \quad \text{on } \Gamma^{m}_e
\]  

(7.38)

\[
d = 0 \quad \text{on } \Gamma^{f}_e
\]  

(7.39)

where \( d(x, t) \) is the function used to compute the displacement of the nodal coordinates, \( g(x, t) \) is the displacement of the free surface, \( \Gamma^f_E \) is the part of the boundary that is fix, and \( \Gamma^m_E \) is the free surface boundary.

The parameter \( \alpha^e \) controls the manner in which the elements deform. Larger elements are assigned a lower value of \( \alpha^e \) than smaller elements. Therefore, the largest elements absorb most part of the deformation of the mesh, and as a consequence, the method can accommodate large displacements of the free surface without having to re-compute the mesh. The value of \( \alpha^e \) depends on the volume \( V_e \) of element \( e \), the volume of the smallest element of the mesh \( V_{\text{min}} \), and the volume of the largest element of the mesh \( V_{\text{max}} \) as follows:
\[ \alpha^e = \frac{1-V_{\text{min}}/V_{\text{max}}}{V_{\text{e}}/V_{\text{max}}} \] (7.40)

7.4 Numerical results

A literature review reveals that there are no well-established simple benchmark problems for validating turbulence models that have free surfaces. A problem that is becoming popular and could serve as benchmark problem for turbulence models is the 3D dam break problem, which consists of a column of fluid that is initially at rest. This column of fluid collapses due to the effects of gravity, and spreads throughout the computational domain creating a free surface that evolves rapidly and even changes its topology. There are several variations of the problem, which can also include obstacles that interfere with the spreading fluid. Although this problem is suitable to show that a method can represent flows with large free surface deformations, it cannot be used to study the numerical attributes of the turbulence models employed because the modeling of the free surface is a major source of numerical error.

Despite the lack of simple benchmark problems for turbulent free surface flows, there are some widely used benchmark problems for turbulence models on fix domains. On the other hand, there are also well-established benchmark problems for laminar flows with free surfaces. A popular example of the first type of flow is the confined turbulent channel flow, which consists of a fluid driven by a body force. The flow is confined by two parallel fixewalls. Reference DNS results were established by Moser and co-workers [103] for various Reynolds numbers. Numerical models for problems with laminar free surface flows are typically tested using sloshing benchmark problems. These problems typically consist of a tank filled with fluid that is subjected to a periodic lateral acceleration or body force [84, 83]. To avoid numerical problems in the definition of the wetting surface, slip boundary conditions are generally applied in the interface between the fluid and the fix walls. Due to the imposition of the slip boundary condition, there are no boundary layers that generate vertical structures, and therefore, the flow in sloshing problems is rarely turbulent.

In this section we present two types of numerical tests that, due to their simplicity, can potentially become standard benchmark problems for evaluating the performance of turbulence models for problems with free surfaces. First we consider a turbulent channel that
only has a fix wall on the bottom, while the top boundary is a free surface. The flow, which is subjected to a gravity force, is studied at $Re_T = 395$ using two different slopes of the bottom boundary. The second problem is inspired by [136, 7], and consists of an open channel flow with a non-flat bottom surface. We use the same settings as the ones used in [136]. We compare the results with experimental data reported in [7] and LES results reported in [136]. This test, in addition to show the applicability of the present method, also shows its accuracy. For this second problem, we also consider a configuration that has a more complex free surface than the one reported in [136].

All the numerical tests have been conducted using tri-linear hexahedral elements for the coarse-scale fields, quadratic bubble functions for the fine-scale level-I fields and quartic bubble functions for the level-II velocity field. The element integrals have been evaluated using full Gaussian quadrature, and the semi-discrete formulation has been discretized in time using the generalized-alpha method, with $\rho_\infty = 0$.

### 7.4.1 Flat open turbulent channel flow

The confined channel flow is a widely used benchmark problem due to the existence of a DNS solution [103]. The flow has a boundary layer on the vicinity of each of the two plane walls, and the flow is chaotic in between the two walls. In this problem, the chaotic motion of the flow results in a nonzero local flux across the fictional mid-height plane parallel to the walls. The nonzero local fluxes motivate the present problem. If we only study half channel, and the former mid-high plane is considered to be a free surface, the resultant flow has an evolving free surface that is driven by the chaotic motion of the flow. Therefore, this problem involves a turbulent flow that interacts with a free surface. The flat open channel flow has been previously studied by Pan and Banerjeea [112] and Nagaosa [104]. However, in the previous studies, the free surface was treated as a rigid wall with free-slip boundary condition, which precludes the deformation of the free surface.

The computational domain studied is schematically represented in Fig. 7.1. The length of the domain is 6, its width 4, and its height 1. We apply zero velocity on the bottom face, periodic boundary conditions on the lateral faces, and the top face is considered to be a free surface. The viscosity of the fluid is set equal to 0.0001472. The problem is driven by a
constant body force. First we consider \( f_x = 0.00337204 \) and \( f_y = 0.2697632 \), which is equivalent to setting the slope of the bottom surface to 1/80. The second flow that we consider has a slope equal to 1/40, and the components of the body force are set to \( f_x = 0.00337204 \) and \( f_y = 0.134882 \). The Reynolds number of the flow based in Taylor’s micro-scales [113] is 395 in both cases.

We study the flow using three meshes of \( 32 \times 32 \times 32 \), \( 64 \times 32 \times 64 \) and \( 64 \times 64 \times 64 \) hexahedral elements. The elements are uniformly distributed in the \( x \) and \( z \) directions and graded on the \( y \) direction. The grading is obtained using a hyperbolic distribution that clusters more nodes near the bottom wall and is given by the following expression:

\[
y_i = 1 - \frac{\tanh(\gamma (1 - i/N))}{\tanh(\gamma)}
\]  

(7.41)

where \( \gamma \) is set to 1.5 for all the cases, \( N \) is the number of elements in the wall-normal direction, and \( i \in [0, N] \). The time step size \( \Delta t \) is set to 0.025 for all the cases.

The flow is initialized with a stream-wise parabolic velocity field that is randomly perturbed in the \( x \) and \( z \) directions by a quantity that is less than 10\% of the parabolic mean velocity. After a transitory regime in which the turbulence structures develop and the free surface starts to evolve, the flow reaches a statistically steady state. Then the solution field is sampled every 10 time steps for a period of 5000 time steps. The sampled solution is averaged over time and also in the stream-wise and span-wise directions. For the flow with the highest slope, Fig. 7.2 shows the geometry of the problem and the velocity field at an instant of time.

Figure 7.3 shows the mean velocity and the root mean square value of its fluctuations in each of the three spatial dimensions. In addition to show the results obtained with each of the meshes employed, Fig. 7.3 also shows the DNS results of the equivalent confined turbulent channel flow [103]. Near the wall, the statistics of the confined channel are very similar to the statistics of the open channel. This is due to the fact that the effects of the free surface are small far away from the free surface. Closer to the free surface, the results of the confined channel are different from the results of the open channel because the effects of the free surface are more significant. The effect of the free surface is clearly noticeable in the fluctuations of the velocity field in the wall-normal and span-wise directions, i.e., Fig. 7.3(c)
and Fig. 7.3(d), respectively. All the results presented in Fig. 7.3 are expressed employing wall units [113]. The first column of Table 7.1 shows the Froude number of the flow, which is a measure of the ratio between inertial and gravity forces, and is defined as:

$$Fr = \frac{U_o}{\sqrt{f_s L_y}}$$  \hspace{1cm} (7.42)

where $U_o$ is the mean velocity of the free surface.

The same study was also performed for the case of the channel with stepper slope. Figure 7.4 shows the statistics of the flow, in which the same conclusions as the previous case can be drawn. While near the wall the results are very similar to the statistics of the confined turbulent channel, the effects of the free surface are more noticeable on the top part of the channel. The second column of Table 7.1 shows the Froude number obtained with each of the meshes. As expected, Froude number is higher than in the previous case because the channel is steeper, and thus, the inertial force is more significant than in the previous case.

### 7.4.2 Wavy open turbulent channel flow

The second type of flow that we study is also an open channel flow, but in the present Section, the channel is not flat. The bottom of the channel has a shape that resembles a fixed sand dune. The problem was proposed by Balachandar and Patel [7], who studied deep water flows experimentally, and Yue and co-workers [136], who studied the problem computationally. We study the same problem and compare our results with the existing data. Additionally, we also study the same flow at higher Froude number to show the applicability of the present method to problems in which the free surface is subjected to larger deformations.

The computational domain employed in our studies is schematically represented in Fig. 7.5, and the precise coordinates of its key sections are defined in Table 7.2. The bottom boundary has the shape of a sand dune. Zero velocity is prescribed on the bottom boundary. On the lateral walls, periodic boundary conditions are applied. The top boundary is located at a distance $L$ from the crest of the dune and is considered to be a free surface. The viscosity of the fluid is set equal to 1.
With the goal of comparing our results with existing data [136, 7], we set $L=132$, and we apply a body force of magnitude 981. The force is inclined such that its components are $f_x=0.7651799$ and $f_y=-980.9997$. The domain is discretized using $80 \times 64 \times 64$ hexahedral elements that are evenly distributed in the $x$ and $z$ directions. As shown in Fig. 7.6, the elements are graded in the $y$ direction. The top 5 layers of elements have a height of $4/5$, the remaining elements are distributed using an hyperbolic function with $\gamma=1.75$. The time step size $\Delta t$ is set to 0.015.

The problem is initialized from rest and is let to evolve until it reaches a statistically steady state. Figure 7.7 shows the developed velocity field. It can be seen that, for the present flow conditions, the motion of the free surface is very small. To compute the statistics of the flow, we sample the solution every 10 time steps in an interval of 5,000 steps. In addition to average the solution over all the sampled time steps, we average it along the span-wise direction. Figure 7.8 shows the averaged geometry, the mean velocity field, and a few uniformly distributed velocity streamlines. The mean flow has a recirculation zone downstream of the dune, which starts at $x=10$ and end at $x=104$. The end of the recirculation zone agrees well with the LES result reported by Yue and co-workers [136], $x=100$. The Froude number based on the mean velocity of the free surface at $x=0$ is 0.42. Figure 7.9 shows the mean velocity of the flow along 6 vertical sections of the channel. The results are compared with the experimental data reported by Balachandar and Patel [7] and the results obtained by Yue et al. [136] employing a dynamic Smagorinsky model and a similar mesh. The results agree very well with the existing data. The LES results [136] are plotted beyond $y/L=1$ because they considered a layer of air on top of the open channel. The results show that the layer of air, which adds a small amount of inertia to the free surface, does not have a significant effect on the results in the case of the studied flow. Figure 7.10 shows the root mean square of the fluctuations of the velocity field in the stream-wise direction at several sections. In this case, a reasonably good agreement with previously published results is also observed.

To show the applicability of the present method to problems that undergo larger deformations of the free surface, we study the wavy channel at a higher Froude number. We consider a shallower flow by setting $L$ equal to 20, and a steeper mean inclination of the
channel bottom. The new slope is obtained by setting the body force to \( f_x = 4.0 \) and \( f_y = -980.992 \). The other parameters of the problem are the same as in the previous flow.

The mesh employed in the present test has been designed following the same guidelines as in the previous case. However, now we consider a mesh that consists of \( 80 \times 54 \times 48 \) elements. The time step size is set equal to 0.01. Figure 7.11 shows the velocity field once the flow is completely developed. The averaged solution is represented in Fig. 7.12, in which the streamlines of the velocity field also show the presence of a recirculation region downstream of the dune. The Froude number of the flow is 0.69. Vertical profiles of the stream-wise velocity field and its fluctuations are represented in Figs. 7.13 and 7.14, respectively.

### 7.5 Conclusions

We have extended our previous work on residual-based turbulence models for problems with moving boundaries [100] to a formulation that is able to accommodate free surface problems. Using the VMS framework, the method has been derived assuming a multiscale decomposition of the velocity and pressure fields in coarse and fine scales. This has led to two coupled mixed-field problems. The mixed-field fine-scale problem has been stabilized by assuming a further decomposition of the velocity field in fine-scales level-I and level-II. The problem that governs the level-II scales has been modeled using fourth order bubble functions, and its solution has been variationally projected in the problem that governs the level-I scales. The stabilized level-I scale problem has been solved using quadratic bubble functions. Level-I model has been employed to approximate the fine-scale fields and has been variationally projected to the coarse-scale problem to model the effects of the sub-grid scales on the resolved scales. The bubble functions approach employed to model the two fine-scale problems has led to a formulation that does not have any embedded or tunable parameters. The formulation has been applied to study two problems with simple geometry in order to show the applicability of the method. The first problem considered is a flat open channel with a fix boundary on the flat bottom, and a free surface on the top boundary. The flow is driven by an inclined body force. Two different inclinations of the body force have been considered. The long term solution of the problem is a statistically stationary flow. The mean velocity field and its root mean square fluctuations have been reported over the depth of the channel. The second problem studied is similar to the previous problem. It is an open channel flow.
with a wavy bottom boundary. Two different configurations of the channel have been studied, and the results obtained for the first one have been compared with the experimental and numerical results reported by [7] and [136], respectively. The numerical tests have showed the accuracy and the versatility of the proposed formulation for studying free surface flows.

7.6 Figures and tables

![Figure 7.1](image1.png) Schematic diagram of the channel problem with a flat bottom

![Figure 7.2](image2.png) Instantaneous velocity field of the highest slope channel
Figure 7.3 Low slope channel. (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions.
Figure 7.4 High slope channel, (a) Mean stream-wise velocity. R.M.S. velocity fluctuations in: (b) the stream-wise, (c) the wall-normal and (d) the span-wise directions
Figure 7.5 Schematic diagram of the channel problem with a wavy bottom

Figure 7.6 Transversal view of the mesh of the wavy channel flow with L=132
Figure 7.7 Instantaneous velocity field for L=132

Figure 7.8 Mean velocity field for L=132
Figure 7.9 Mean velocity along the y-coordinate for L=132, (a) x=40, (b) x=80, (c) x=100, (d) x=120, (e) x=240 and (f) x=360
Figure 7.10 R.M.S. fluctuations of the stream-wise velocity field along the y-coordinate for $L=132$, (a) $x=40$, (b) $x=80$, (c) $x=100$, (d) $x=120$, (e) $x=240$ and (f) $x=360$
Figure 7.11 Instantaneous velocity field for $L=20$

Figure 7.12 Mean velocity field for $L=20$
Figure 7.13 Mean velocity along the y-coordinate for $L=20$, (a) $x=40$, (b) $x=80$, (c) $x=100$, (d) $x=120$, (e) $x=240$ and (f) $x=360$
Figure 7.14 R.M.S. fluctuations of the stream-wise velocity field along the y-coordinate for L=20,
(a) x=40, (b) x=80, (c) x=100, (d) x=120, (e) x=240 and (f) x=360
Table 7.1 Froude number of the flat open channel flow

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Lowest slope</th>
<th>Highest slope</th>
</tr>
</thead>
<tbody>
<tr>
<td>32×32×32</td>
<td>2.68</td>
<td>3.87</td>
</tr>
<tr>
<td>64×32×64</td>
<td>2.39</td>
<td>3.46</td>
</tr>
<tr>
<td>64×64×64</td>
<td>2.37</td>
<td>3.34</td>
</tr>
</tbody>
</table>

Table 7.2 Coordinates of key locations of the bottom of the wavy channel

<table>
<thead>
<tr>
<th>x-coordinate</th>
<th>y-coordinate</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>Periodic boundary</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>Change of slope</td>
</tr>
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<td>50</td>
<td>-20</td>
<td>“</td>
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<tr>
<td>75</td>
<td>-20</td>
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<td>“</td>
</tr>
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<td>325</td>
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</tr>
<tr>
<td>390</td>
<td>0</td>
<td>“</td>
</tr>
<tr>
<td>400</td>
<td>0</td>
<td>Periodic boundary</td>
</tr>
</tbody>
</table>
Chapter 8

Implementation and performance of the computer code

8.1 General considerations

Due to the relative high computational cost of solving the Navier-Stokes equations, the mathematical formulations developed in Chapters 2-7 have been implemented in a parallel computer code. In this Chapter we describe the implementation details, and we study the performance of the developed computer code.

Since the Navier-Stokes equations are transient and nonlinear, the developed semi-discrete formulations proposed in Chapters 2-7 must be discretized in time and an iterative scheme needs to be applied to solve the nonlinearity. The approach adopted to obtain a numerical solution is based on the generalized alpha method, which discretizes the problem in time. The resulting nonlinear systems of equations are solved employing a Newton-Krylov-Schwarz strategy. The Newton method is employed to iteratively solve the algebraic nonlinear problems, and the stabilized bi-conjugate gradient method is used to solve the linear systems of equations, which are pre-conditioned with an additive Schwarz scheme.

A significant characteristic of the presented formulations is that the computation of the fine-scale fields and the element contributions to the tangent matrices and residual vectors are done at the element level. This makes the algorithms highly amenable for parallel implementation.

The developed code has been built on top of the standard finite element program FEAP [121], which is used to perform the standard tasks of the finite element method. The parallel implementation is done using the standard Message Passing Interface (MPI). To solve the linear systems of equations we use PETSc [8]. This makes the resulting code portable across different distributed-memory computers.

In the following sections we analyze the three aspects that need to be taken into account in order to develop an efficient scalable computer program [4]. These are the scalability of the algorithm, the per-processor performance, and the scalability of the
implementation. In Sec. 8.2, we discuss the strategy that leads to a scalable algorithm. In the following section, we study the per-processor performance and we discuss implementation details that improve the efficiency of the cache memory. The parallel performance of the implementation is studied in Sec. 8.5. Although the performance studies are conducted with the formulation developed in Chapter 5, similar results are expected for the other proposed formulations.

The performance studies have been conducted on Trestles, which is a computing system supported by the XSEDE program of the National Science Foundations, and is managed by the San Diego Supercomputing Center. The cluster has 324 compute nodes. Each of the nodes has 4 sockets with 8-core 2.4 GHz AMD Magny-Cours processors. Each node has 64 GB of RAM, and they are interconnected with a Voltaire QDR Infiniband.

### 8.2 Parallelization strategy

The developed formulations are amenable for parallel implementation because most of the computations can be done at the element level. To parallelize the proposed algorithms we employ a domain decomposition technique that assigns a part of the elements of the mesh to each processor. The nodal points are assigned to the same processor that hosts the elements that are connected to the node. The nodes that are connected to elements that are hosted by two or more processors are only assigned to one of the processors, and a copy of the nodal information is given to the other processors that need the nodal data to perform the element-level computations. This “ghost” node approach allows performing all the element-level computations locally without the need of communicating data between processors. Thus, the element tangent matrices and residual vectors are computed by the local processor, and then they are assembled to the corresponding equations of the global system of linear equations. In general, the element contributions are assembled to equations that belong to the same processor that computes the contribution. However, on the boundaries of the partitions, there are elements that contribute to equations that are located at the local processor and equations that are located at neighboring processors. This issue can be treated by communicating the data to the appropriate processor. Although this is a valid approach, it has an evident overhead due to the communication cost. A second approach that can be adopted is to compute the element quantities in a redundant manner so that no communication is needed. In the present
code, we have employed the second approach because the additional computational cost associated with the redundant computations is small compared to the cost of computing the contributions of all the other elements. Figure 8.1 shows a schematic representation of the partitioning of mesh in two parts. As it can be seen, the elements that are on the shared boundaries of the partitions are computed twice. Figure 8.2 shows the actual partitioning of a mesh.

To partition the meshes we use Metis [76], which is a library that provides several options for the decomposition of the domain. In one of the options, the meshes can be decomposed in domains that approximately have the same number of elements. In this case, the mesh partitioning algorithm also tries to minimize the number of nodes that lie on the interface between partitions. A second option offered by Metis [76] is the partitioning of the mesh prioritizing the minimization of the number of nodes that lie on partition boundaries. While the first approach prioritizes work balance between processors, the second approach prioritizes the minimization of communication between the processors. We have noticed that some of the partitions obtained with the first approach have rough boundaries that turn out to be bottlenecks of the overall computation flow. Additionally, these rough boundaries degrade the efficiency of the pre-conditioner, which results in an increase of the number of iterations that the Krylov solver needs. We have observed that the overall computational cost of solving a problem with the second approach can be up to 16% lower than the cost of the first approach. Thus, all the results reported in the following sections have been conducted with meshes partitioned with the second approach.

The computation of element quantities is done locally, and therefore there is no communication in this part of the algorithm. In addition, the “ghost” elements approach circumvents the need of communication between processors during the assembly of the global matrices and vectors. As a consequence, the solution of the linear systems of equations and the convergence checks are the only parts of the algorithm that require communication between processors. The communication events can be classified in two classes. The first class consists of all-to-all and all-to-one operations such as MPI_AllReduce. These events involve message-passing between all the processors. The second class consists of point-to-point operations such as MPI_Send and MPI_Receive, which only involve communication between pairs of processors that have a common partition interface. In the present
parallelization approach, the communication pattern of point-to-point operations is determined by the partitioning of the mesh. Figure 8.3 shows the point-to-point communication pattern of the mesh represented in Fig. 8.2, which is partitioned using the Metis [76] scheme that minimizes interfaces between partitions. It can be seen that some processors communicate to a higher number of processors than others. In addition, there is no set of processors that is loosely connected to another set. The partitioning scheme employed balances the computation work and minimize overall communication. However, the scheme does not balance the communication pattern, i.e. some processors have to send and receive more messages than others. Another limitation of the mesh partitioning scheme is that it does not take advantage of the different bandwidth between the intra-nodal and the inter-nodal networks. These two facts, may introduce load unbalancing in the code. An improved mesh partitioning scheme would take advantage of the architecture of the computing system, and would balance both the computing work and the communication pattern.

8.3 Per-processor performance

In this section we study the per-processor performance, which is one of the most important aspects for achieving a good overall performance of a parallel computer code. To study the per-processor performance we use the PETSc [8] profiling tools, which not only measure the performance of PETSc [8] functions, but they can also be used to measure the performance of user-written subroutines. We also use Jumpshot-4 [23] and PFMPI-2.1 [50].

One of the most important parts of the code is the set of subroutines that perform the element-level calculations. To attain a good per-processor performance in these set of subroutines, the Gauss quadrature loops, which are the most computationally expensive, are optimized to improve data locality. In addition, the expressions employed to compute the element tangent matrices and residual vectors are implemented using a symbolic algebraic manipulator. The use of the symbolic manipulator circumvents the need for some for-loops that would introduce an overhead to the program. In addition, it minimizes the required number of floating point operations.

The linear systems of equations are solved employing PETSc [8], which also provides the interface to test different linear solvers and pre-conditioners. To optimize the performance of PETSc [8], structural blocking is employed, and we take into account that each node of the
mesh has 4 degrees of freedom. This helps improving the cache performance by reducing the number of loads and stores.

To characterize the per-processor performance of the code, we consider a turbulent channel flow at \( \text{Re} = 395 \). The dimensions of the computational domain are \( 2\pi \) in the longitudinal direction, \( 2 \) in the wall-normal direction, and \((2/3)\pi\) in the span-wise direction. No-slip boundary condition is applied on the two walls, while periodic boundary conditions are applied on all the other faces of the domain. The domain is discretized using \( 32 \times 32 \times 32 \) hexahedral elements that are evenly distributed in the longitudinal and span-wise directions, and are stretched following a hyperbolic distribution in the wall-normal direction. The time step size is set to 0.025. The problem is initialized with a perturbed parabolic velocity field and is let to evolve until it reaches the statistically steady state regime.

The metrics of the code are collected during the solution of 200 time steps of the fully developed flow. Table 1 shows a summary of some of the most important tasks of the code. The amount of time spent on the element loop, which forms and assembles the element tangent matrices and residual vectors, is 58% of the total time. Solving the linear systems of equations takes about 32% of the total time. The remaining part of the time, the code performs other tasks such as convergence checks; it initializes new time steps and writes the solution to the output files. Most of the time spent in the element loop is consumed by the integration loop that computes the element tangent matrices and residuals vectors. Thus, optimizing the integration loop is important to achieve a good overall performance.

The “ghost” node approach adopted in the present work facilitates the assembly of element quantities to the global system of equations because no communication is needed. Therefore, PETSc functions that communicate matrix and vector entries in the assembly stage (i.e., MatAssemblyBegin, MatAssemblyEnd, VecAssemblyBegin and VecAssemblyEnd) only need to be invoked to fulfill the PETSc’s syntax requirements [8]. As a result, they do not perform any operation in the present code.

An important aspect that affects the efficiency of any code is the performance of the functions that invoke all-to-all communication operations (e.g., VecDot, VecDotNorm2, VecNorm). The table shows that the speed achieved in these functions is significantly lower than the speed of other parts of the code. This is a consequence of the poor communication
balance induced by the partitioning. It is important to note that for the partitioning scheme that prioritizes an equal distribution of elements across all the processors, the speed of these functions is of the order of 300Mflop/s.

8.4 Parallel performance

Some computer programs that have a high per-processor performance do not scale well because either the algorithm is not scalable or the communication costs are too high and contribute significantly to the overall computational cost. The domain decomposition approach adopted here results in a scalable algorithm that minimizes the communication between processors. However, for meshes with low number of nodes compared to the number of partitions employed to solve the problem, the number of “ghost” nodes may be very high. In those cases, the redundant work done at the element level may be significant. In this section we study the parallel performance of the code employing meshes of different size.

To perform the scalability study we consider a similar turbulent channel flow to the one studied in Sec. 8.3. We solve the problem employing meshes that consist of $32 \times 32 \times 32$, $128 \times 32 \times 64$ and $256 \times 32 \times 128$ hexahedral elements. For each of the meshes, the problem is solved using different number of processors. In all the cases, the number of elements in the wall-normal directions is the same. The dimension of the channel in the mean stream-wise and span-wise directions is adjusted so that the size of the elements in these two directions is the same for the three meshes. Since the level of resolution of the flow features is the same for the three meshes, the difficulty of solving the nonlinearities is independent of the mesh employed. Thus, the three sets of performance results are comparable. We compute the solution for 50 time steps. A sufficient high number of time steps makes the cost of initialization of the algorithm negligible compared to the cost of computing the actual solution.

It is not possible to solve the problem with the largest number of nodes using a single processor. Therefore, the study is based on the metrics obtained from a run executed with 8 processors.

Figure 8.4 shows the speed-up curves obtained for the three meshes considered in the present study. The speed-up obtained for the meshes studied is quasi-optimal for the cases in which the number of elements is large compared to the number of processors used to solve the problem. Good scalability is achieved while the number of nodes per processor is higher than
As the number of processors employed is increased, the number of equations per processor decreases. As a consequence, the relative communication cost and the number of “ghost” elements and nodes increases because the size of the interface between partitions also increases. To illustrate the importance of “ghost” nodes in the scalability of the code, Fig 8.6 shows the relative number of “ghost” nodes as a function of number of partitions. For the worst case considered, the number of “ghost” nodes is about 70% of the number of actual nodes.

A factor that could negatively affect the scalability of the code is the efficacy of the pre-conditioner. This could happen because the Additive Schwarz pre-conditioner employed in the present study ignores the contribution of the off-processor values of its matrices. Although this reduces significantly the amount of communication required per iteration of the Krylov solver, ignoring the off-processor values could increase the number of required iterations as the number of processors used is increased, and as a result, it could increase the overall computational cost. Figure 8.6 shows that this is not the case as the number of iterations required by the Krylov solver to converge to a tolerance of $10^{-10}$ is independent of the number of processors used to solve the problem. Therefore, ignoring off-processor entries of the pre-conditioner is beneficial even when a large number of processors are used to solve the problem.

Similar parallel performance of the code has also been observed in other parallel computers, including Taub, which is managed by the Computational Science and Engineering program of the University of Illinois at Urbana-Champaign, Abe of the National Center for Supercomputing Applications, Ranger of the Texas Advanced Computing Center, and Kraken of the National Institute for Computational Sciences.

8.5 Conclusions

The formulations presented in Chapters 2-7 are amenable for parallel implementation because the computation of the fine-scale fields is done locally, and as a result, most of the computations are done at the element level. To study the efficiency and the scalability of the proposed algorithms, in the present Chapter we have studied several aspects of the developed parallel computer code. The study has been performed for the three-scale model developed in Chapter 5, which is the most sophisticated turbulence model presented in this dissertation.
We have studied the three aspects that influence the overall efficiency of a parallel computer code. First we have explained the domain decomposition approach that has led to scalable algorithms. This has been achieved using a “ghost” node approach, in which the contribution of the elements that are located on the boundaries of the mesh partitions is computed at each neighboring processor. This requires some redundant computation work, but circumvents the need of communication between processors during the calculation and assembly of the local matrices and vectors to the global linear system of equations. The second aspect of the code that has been analyzed is the per-processor performance. Special emphasis has been given to the subroutines that compute the element contribution to the linear systems of equations. This is where most of the computing time is spent, and therefore, a small inefficiency at these subroutines could dramatically degrade the overall performance of the code. The third aspect of the code that has been studied is the parallel performance. Via a scalability study, we have shown that for systems that are large enough, the code scales well at least for 512 processors.

Although the good overall performance of the code, we have noticed that its scalability is partially constrained by the limitations of the current generation of mesh partitioning algorithms. A limitation of the employed mesh partitioning scheme is that it does not account for the heterogeneous structure of multi-core clusters. Taking into account the different bandwidth between cores would improve the scalability of the code. A second limitation of the mesh partitioning algorithm employed in the present work is that it minimizes the amount of communication between processors, but it does not balance the communication pattern. Therefore, an algorithm that balances the communication would also contribute positively to the scalability of the code.

In conclusion, the proposed algorithms for modeling incompressible turbulent flows are amenable for efficient parallelization, and the developed implementation is efficient and highly scalable.
8.6 Figures and tables

**Figure 8.1** Schematic representation of the mesh partitioning technique

**Figure 8.2** Partitioning of a hexahedral domain that consists of $32 \times 32 \times 32$ elements in 48 partitions. Two of the partitions are highlighted
Figure 8.3 Communication pattern for the partition represented in Fig. 8.2

Figure 8.4 Speed-up
Figure 8.5 Relative number of “ghost” nodes

Figure 8.6 Number of iterations of the linear solver
<table>
<thead>
<tr>
<th>Function</th>
<th>Relative cost</th>
<th>Mflop/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Element loop</td>
<td>58%</td>
<td>-</td>
</tr>
<tr>
<td>Integration loop</td>
<td>38%</td>
<td>42550</td>
</tr>
<tr>
<td>MatMult</td>
<td>8%</td>
<td>28676</td>
</tr>
<tr>
<td>MatSolve</td>
<td>12%</td>
<td>32860</td>
</tr>
<tr>
<td>MatAssemblyBegin</td>
<td>0%</td>
<td>-</td>
</tr>
<tr>
<td>MatAssemblyEnd</td>
<td>0%</td>
<td>-</td>
</tr>
<tr>
<td>VecDot</td>
<td>1%</td>
<td>1123</td>
</tr>
<tr>
<td>VecDotNorm2</td>
<td>1%</td>
<td>1184</td>
</tr>
<tr>
<td>VecNorm</td>
<td>1%</td>
<td>1356</td>
</tr>
<tr>
<td>VecAssemblyBegin</td>
<td>0%</td>
<td>-</td>
</tr>
<tr>
<td>VecAssemblyEnd</td>
<td>0%</td>
<td>-</td>
</tr>
<tr>
<td>KSPSolve</td>
<td>32%</td>
<td>29689</td>
</tr>
<tr>
<td>PCApplied</td>
<td>14%</td>
<td>27920</td>
</tr>
</tbody>
</table>
Chapter 9

Concluding remarks and future directions

9.1 Concluding remarks

This dissertation has presented a series of formulations of increasing degree of sophistication to model a wide spectrum of incompressible flow problems. All the models have been derived using the Variational Multiscale (VMS) framework, in which the solution fields are decomposed in coarse and fine scales. The coarse scales are represented by the finite element discretization, while the fine scales, which are filtered out by the mesh discretization, are modeled in as a function of the residual of the Euler-Lagrange equations for the coarse scales. The fine-scale models are variationally embedded in the problem that governs the coarse scales, resulting in a formulation for the coarse scales that fully accounts for the effects of the fine scales. The overlapping additive decomposition of the solution fields and the derivation of the fine-scale models have given raise to the option of making several modeling assumptions and simplifications. The attributes of the methods have been studied and discussed throughout the dissertation. The formulations have also been cast in an Arbitrary Lagrangian-Eulerian framework to accommodate problems with moving boundaries such as fluid-structure interaction and free-surface problems.

The main conclusions of the present work are the following:

- The hierarchical multiscale approach presented in the dissertation models the effects of the scales that cannot be represented by the finite element discretization, and therefore yields highly accurate schemes for unstructured meshes.

- The proposed turbulence models are governed by fine-scale problems that are driven by the Euler-Lagrange equations for the coarse-scale fields, and they automatically adapt to the flow type (i.e. laminar, transitional and turbulent flows are modeled using the same formulation).

- The fine-scale problems are modeled using a bubble functions approach. This has yielded models that do not have embedded or tunable parameters. As a
consequence, the derived methods can be applied to study any incompressible flow without a-priori knowledge of the flow regime.

- In the cases where the interpolation employed for the coarse-scale fields is able to exactly represent all the features of the flow, the fine-scale models vanish. This is a consequence of the mathematical consistency of the proposed models.

- The effects of assuming a multiscale decomposition of the pressure field, which leads to a \( \text{div} \)-stabilization term, has been explored in Chapter 4. It has been observed that the consideration of a fine-scale pressure reduces the numerical error in the local enforcement of the mass conservation equation.

- In Chapter 4, we have numerically studied the effects of considering orthogonal fine-scales, and thus the effects of ignoring the viscous-type contribution on the weighting slot of the terms that models the effects of the fine scales in the coarse-scale problem. Since the consideration of orthogonal fine-scales is not a required assumption to derive the fine-scales models, we have not made this assumption in any of the models.

- The modeling of the fine-scales problem gives rise to the definition of a non-diagonal second order tensor \( \tau \). In Chapters 4 and 5 we have numerically shown that the diagonalization of the tensor does not have an impact on the computed results. This simplification of the fine-scale model yields a substantial reduction of the computational cost.

- For the case of laminar flows, the fine scales have been considered quasi-static, and therefore their dynamical effects have been neglected. However, to accurately model turbulent flows, the fine-scale velocity has to be considered time-dependent.

- An important simplification that can be done to the time-dependent fine scales is to ignore the contribution of the time-history terms but retain the dependence on the time step size \( \Delta t \). The simplified model presented in Chapter 4 has a pathologic behavior for very small time step sizes. This issue is addressed via the more mathematically sophisticated models presented in Chapters 5-7.

- The derived turbulence models are easy to implement in existing finite elements codes. The only parts of the existing code that need to be modified are the
functions that compute the element consistent matrices and residual vectors. Details on how to implement the element matrices and vectors have been given in Chapter 8 and Appendix A.

- The local character of the fine-scales fields makes the formulation amenable for parallel implementation because most of the computations are done at the element level.

- A performance study of the developed computer code has been presented in Chapter 8. The study discusses the parallelization strategy, the per-processor performance of the code, and its parallel scalability.

- An extensive set of numerical tests have shown that the proposed formulations have good numerical attributes and are applicable to a wide range of problem types, including problems with moving boundaries such as fluid-structure interaction and free surface problems.

9.2 Future research directions

The dissertation has presented a methodology to derive turbulence models for the incompressible Navier-Stokes equations. The derived framework can be further exploited to enlarge the range of applicability of the proposed formulations.

In the present dissertation, the problems that govern the fine scales have been solved using quadratic and fourth order polynomial bubble functions. More sophisticated models that represent the effects of the fine-scale more accurately can be derived. This would enable the use of coarser meshes. In these formulations, more computational effort would be directed at the fine-scales level, and as a consequence, this would improve the performance of the code on massively parallel platforms.

The formulations can be readily extended to model compressible and chemically-reacting fluid flows. Developments in this direction would enable the method to be used for modeling combustion problems.

The presented methods can be employed to study free surface flows that do not contain breaking waves. The combination of the proposed formulations with an interface-capturing technique to represent the free surfaces would make the methods applicable to free
surface flows with breaking waves. In addition, an interface-capturing technique would automatically extend the applicability of the formulation to multi-phase flow problems.
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Appendix A

Details of the formulation implementation

The turbulence model presented in Sec. 5.3.2 can be implemented in an existing finite element code. The only subroutines that need to be modified in a standard finite element code are the ones where the element tangent matrix $K_{ij}^e$ and the element residual vector $R_i^e$ are computed ($i$ and $j$ are local node numbers of an element $e$).

In this appendix we present the details to implement the formulation in an efficient manner. For the sake of simplicity, the model that neglects the time history of the fine scales and employs a diagonalized stabilization tensor is considered. The code to be used to compute the tangent matrix and residual vectors can be generated by employing an algebraic symbolic manipulation tool.

Let $N_i = N_i(x, y, z)$ be the shape function associated with node $i$, $v = (v_x, v_y, v_z)$ the computed velocity field, $v' = (v'_x, v'_y, v'_z)$ the fine scale velocity field, $f = (f_x, f_y, f_z)$ the external body force, $\nu$ the viscosity of the fluid and $\tau$ the second order tensor defined in equation (5.41) of Sec. 5.3.1. We can define the matrices to be used to generate $K_{ij}^e$ and $R_i^e$ as follows:

- Velocity operator:

$$V_i = N_i I_{3x4} \quad (A.1)$$

where

$$I_{3x4} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad (A.2)$$
- Pressure operator:
\[ P_i = \begin{bmatrix} 0 & 0 & 0 & N_i \end{bmatrix} \] (A.3)

- External body force:
\[ F = \begin{bmatrix} f_x & f_y & f_z & 0 \end{bmatrix}^T \] (A.4)

- Fine scale velocity:
\[ FS = \begin{bmatrix} v'_x & v'_y & v'_z \end{bmatrix}^T \] (A.5)

- Gradient of the velocity field:
\[ \text{GRADV} = \begin{bmatrix} v_{x,x} & v_{x,y} & v_{x,z} \\ v_{y,x} & v_{y,y} & v_{y,z} \\ v_{z,x} & v_{z,y} & v_{z,z} \end{bmatrix} \] (A.6)

- Diagonalized stabilization tensor for the momentum equation:
\[ T_M = \begin{bmatrix} \tau_{11} & 0 & 0 \\ 0 & \tau_{22} & 0 \\ 0 & 0 & \tau_{33} \end{bmatrix} \] (A.7)

- Stabilization parameter for the continuity equation:
\[ T_C = \tau_{44} \] (A.8)

- Laplacian operator 1:
\[ \text{LAPN}_i = \begin{bmatrix} 2N_{i,xx} + N_{i,yy} + N_{i,zz} & N_{i,xy} & N_{i,xz} & 0 \\ N_{i,xy} & N_{i,xx} + 2N_{i,yy} + N_{i,zz} & N_{i,yz} & 0 \\ N_{i,xz} & N_{i,yz} & N_{i,xx} + N_{i,yy} + 2N_{i,zz} & 0 \end{bmatrix} \] (A.9)
- Laplacian operator 2:

\[
SLAPN_i = \left( N_{i,xx} + N_{i,yy} + N_{i,zz} \right) I_{3 \times 4}
\]  
(A.10)

- Gradient operator of a pressure field

\[
GRADN_i = \begin{bmatrix} 0 & 0 & 0 & N_{i,x} \\ 0 & 0 & 0 & N_{i,y} \\ 0 & 0 & 0 & N_{i,z} \end{bmatrix}
\]  
(A.11)

- Symmetric gradient operator of the velocity field:

\[
SGRAD_i = \begin{bmatrix} N_{i,x} & 0 & 0 & 0 \\ 0 & N_{i,y} & 0 & 0 \\ 0 & 0 & N_{i,z} & 0 \\ N_{i,x} & N_{i,y} & 0 & 0 \\ N_{i,z} & 0 & N_{i,x} & 0 \\ 0 & N_{i,z} & N_{i,y} & 0 \end{bmatrix}
\]  
(A.12)

- Auxiliary tensor employed to compute the standard viscous term:

\[
D = \nu \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}
\]  
(A.13)

- Divergence of the velocity field:

\[
DN_i = \begin{bmatrix} N_{i,x} & N_{i,y} & N_{i,z} & 0 \end{bmatrix}
\]  
(A.14)
- Coarse-scales advection operator:
  \[
  \mathbf{AGRADV}_i = \left( v_x N_{i,x} + v_y N_{i,y} + v_z N_{i,z} \right) \mathbf{I}_{3 \times 4}
  \]  
  (A.15)

- Fine-scales advection operator:
  \[
  \mathbf{FGRADV}_i = \left( v'_x N_{i,x} + v'_y N_{i,y} + v'_z N_{i,z} \right) \mathbf{I}_{3 \times 4}
  \]  
  (A.16)

- Transposed coarse-scales advection operator:
  \[
  \mathbf{AGRADV}_T = \begin{bmatrix}
  N_{i,x} \\
  N_{i,y} \\
  N_{i,z}
  \end{bmatrix}
  \begin{bmatrix}
  v_x & v_y & v_z & 0
  \end{bmatrix}
  \]  
  (A.17)

- Transposed fine-scales advection operator:
  \[
  \mathbf{FGRADV}_T = \begin{bmatrix}
  N_{i,x} \\
  N_{i,y} \\
  N_{i,z}
  \end{bmatrix}
  \begin{bmatrix}
  v'_x & v'_y & v'_z & 0
  \end{bmatrix}
  \]  
  (A.18)

Operators (A.1)-(A.18) can be employed to generate the computer code to be used to compute the integrands for the following matrices and vectors:

\[
\mathbf{\tilde{K}}_{eij} = \int_{\Omega_e} \left( \left( \mathbf{GRADN}_i \right)^T \mathbf{D} \mathbf{GRADN}_j + \left( \mathbf{V}_i \right)^T \mathbf{AGRADV}_j 
\right.
\left. + \left( \mathbf{P}_i \right)^T \mathbf{DN}_j - \left( \mathbf{DN}_i \right)^T \mathbf{P}_j + T_C \left( \mathbf{DN}_i \right)^T \mathbf{DN}_j \right) d\Omega_e
\]  
(A.19)

\[
\mathbf{\tilde{M}}_{eij} = \int_{\Omega_e} \left( \mathbf{V}_i \right)^T \mathbf{V}_j d\Omega_e
\]  
(A.20)
\[
\begin{align*}
\hat{K}_{ij}^e &= \int_{\Omega_e} \left( \nu \text{LAPN}_i + \text{AGRADV}_i - (\text{GRADV})^T V_i ight)^T T \left( -\nu \text{SLAPN}_j + \text{AGRADV}_j \right) + \text{GRADV} V_j + \text{GRADN}_j \\
& \quad + (V_j)^T \text{GRADV} V_j \\
\hat{M}_{ij}^e &= \int_{\Omega_e} \left( \nu \text{LAPN}_i + \text{AGRADV}_i - (\text{GRADV})^T V_i \right)^T T_{M_i} V_j \\
\hat{R}_i^e &= \int_{\Omega_e} (V_i)^T F + \left( \nu \text{LAPN}_i + \text{GRADN}_i + \text{AGRADV}_i \right)^T T_{M_i} V_j \quad \text{FS} \\
\end{align*}
\]

Then the tangent matrix element tangent matrix \( \hat{K}_{ij}^e \) and the element residual vector \( \hat{R}_i^e \) can be obtained as follows:

\[
\hat{K}_{ij}^e = \hat{K}_{ij}^e + \hat{K}_{ij}^e + \frac{\alpha_m}{\alpha_F \gamma \Delta t} (\hat{M}_{ij}^e + \hat{M}_{ij}^e)
\]

where \( \alpha_f, \alpha_m \) and \( \gamma = 1/2 + \alpha_m - \alpha_f \) are the parameters of the generalized alpha method and \( \Delta t \) is the time step size, and the residual vector is computed as follows:

\[
\hat{R}_i^e = \hat{R}_i^e - \sum_{j=1}^{n_{el}} \hat{K}_{ij}^e d_j^e - \sum_{j=1}^{n_{el}} \hat{M}_{ij}^e \dot{d}_j^e
\]

where \( n_{el} \) is the number of nodes in the element \( e \), \( d_j^e \) is a column vector that contains the three components of the nodal velocity and pressure of node \( j \) evaluated at \( t = t_{n+\alpha_f} \), and \( \dot{d}_j^e \) is a 4-dimensional column vector that contains the acceleration of node \( j \) evaluated at \( t = t_{n+\alpha_m} \), and its last component is zero.

**Remark:** For the case of linear tetrahedral elements, all the second derivatives of the shape functions are identically zero, and therefore, the formulation can be simplified to avoid doing operations that are not strictly necessary.