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Volker John

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ON LARGE EDDY SIMULATION AND VARIATIONAL
MULTISCALE METHODS IN THE NUMERICAL SIMULATION OF
TURBULENT INCOMPRESSIBLE FLOWS

VOLKER JOHN, Saarbrücken

Abstract. Numerical simulation of turbulent flows is one of the great challenges in Computational Fluid Dynamics (CFD). In general, Direct Numerical Simulation (DNS) is not feasible due to limited computer resources (performance and memory), and the use of a turbulence model becomes necessary. The paper will discuss several aspects of two approaches of turbulent modeling—Large Eddy Simulation (LES) and Variational Multiscale (VMS) models. Topics which will be addressed are the detailed derivation of these models, the analysis of commutation errors in LES models as well as other results from mathematical analysis.

Keywords: incompressible turbulent flows, Large Eddy Simulation (LES), commutation errors, Variational Multiscale (VMS) methods

MSC 2000: 76F65, 76F02, 65M06

1. INTRODUCTION

This paper is based on lectures given at the *9th School on Mathematical Theory in Fluid Mechanics* held in Paseky (Czech Republic) in June 2005. It is intended for students and researchers who like to get some basic ideas about the difficulties in the simulation of turbulent incompressible flows, about some current approaches of treating them and about some mathematical results connected with turbulent flow simulation. Of course, the whole topic of turbulent flow simulation cannot be treated in a single paper. Every year, a huge number of papers are published which study the aspects of simulation of turbulent flows. The topics presented in this paper are chosen with respect to the scientific interests of the author. A number of monographs is available which present different approaches and provide more details

on the topics presented here, e.g., Mohammadi and Pironneau [45], Lesieur [43], Pope [48], Sagaut [51], the monograph [29] and Berselli, Iliescu and Layton [4].

The paper is organized as follows:

- Section 2. The basic equations for incompressible flows are introduced and physical mechanisms of turbulent flows are explained shortly. These mechanisms lead finally to an estimate of the size of the smallest flow structures in turbulent flows. This estimate tells us that it is by far impossible to simulate the behavior of all structures of a turbulent flow on present-day computers. Only some large structures can be simulated and the influence of the small structures onto the large ones has to be described in a different way—this is the central issue of turbulence modeling.
- Section 3. The classical Large Eddy Simulation (LES), one of the currently most popular approaches in turbulence modeling, is introduced. In this approach, the large flow structures are defined by spatial averaging. The derivation of equations for these large flow structures is based on the assumption of commutation of two operators. This assumption is violated in many situations and some analytical results for commutation errors are presented. Finally, the modeling of the Reynolds stress tensor, which is the central issue of the classical LES, is discussed.
- Section 4. Variational Multiscale (VMS) methods, which define the large flow structures by projection into subspaces, will be introduced. After explaining their basic ideas, a concrete approach by a VMS method will be presented in more detail.
- Section 5. Finally, some concluding remarks will be given.

2. SOME PHYSICAL CHARACTERISTICS OF TURBULENT INCOMPRESSIBLE FLOWS

2.1. The model

Numerical simulation of turbulent incompressible flows is based on the model of the dimensionless incompressible Navier-Stokes equations

$$\begin{aligned}
 (1) \quad \frac{\partial \mathbf{u}}{\partial t} - 2\text{Re}^{-1} \nabla \cdot \mathbb{D}(\mathbf{u}) + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \mathbf{f} & \quad \text{in } (0, T] \times \Omega, \\
 \nabla \cdot \mathbf{u} = 0 & \quad \text{in } (0, T] \times \Omega, \\
 \mathbf{u}(0, \cdot) = \mathbf{u}_0 & \quad \text{in } \Omega.
 \end{aligned}$$

Here \mathbf{u} is the velocity, $\mathbb{D}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ the velocity deformation tensor, p the pressure, \mathbf{f} represents body forces, $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, is a domain and T the end of

a time interval. The Reynolds number Re is defined by

$$\text{Re} = \frac{LU}{\nu},$$

where L [m] is a characteristic length scale, U [m/s] is a characteristic velocity and ν [m²/s] is the kinematic viscosity. If Ω is a bounded domain, (1) has to be equipped with boundary conditions. The first equation in (1) describes the conservation of linear momentum and the second equation the conservation of mass. The derivation of the Navier-Stokes equations (1), based on these conservation principles, can be found in many books on fluid mechanics or hydro-mechanics, e.g., [40], [48].

The Navier-Stokes equations possess one characteristic parameter—the Reynolds number. Turbulent flows are characterized by a high Reynolds number. In applications, the range of the Reynolds number for flows of this type starts around several thousand. Often it is even larger by some orders of magnitude. In the case of high Reynolds numbers, the stabilizing forces in the momentum balance (the viscous term $2\text{Re}^{-1}\nabla \cdot \mathbb{D}(\mathbf{u})$) are small compared to the destabilizing forces (the convective term $D\mathbf{u} = \mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}$, where $D\mathbf{u}$ is the material derivative).

One may ask whether (1) is a correct model for describing turbulent flows. There is not yet an ultimate answer to this question. In the derivation of the Navier-Stokes equations, the following assumptions are made concerning the so-called Cauchy stress tensor, [40]:

- it depends only on the first order spatial derivatives of \mathbf{u} , where in [40] the condition is stated that for this assumption the velocity should be not too large,
- it depends linearly on the first order spatial derivatives of \mathbf{u} .

Flows which obey these assumptions are called Newtonian flows. A question is if these assumptions are valid in the whole range of the Reynolds number or if it is possible that Newtonian fluids behave in a non-Newtonian way for high Reynolds numbers. Also from the mathematical point of view, the Navier-Stokes equations are not yet fully understood. The uniqueness of an appropriately defined weak solution or the existence of an appropriately defined classical solution are an open problem in the (natural) three-dimensional case, [15], [53]. The solution of this problem is currently one of the big challenges in mathematics, [10]. Might it be that this unresolved problem has its origin in an incorrect model? However, the Navier-Stokes equations (1) are currently the best model available for turbulent incompressible flows.

2.2. The size of the smallest scales

There is no clear mathematical definition of what is “turbulence”. From the mathematical point of view, turbulent flows occur at high Reynolds numbers. From

the physical point of view, these flows are characterized by possessing flow structures (eddies, scales) of very different sizes. Consider, e.g., a tornado. This tornado has some very large flow structures (large eddies) but also millions of very small flow structures. For a numerical simulation of turbulent flows, the question on the size of the smallest eddies has to be answered. This size is denoted by λ .

Much of the physical turbulence theory, e.g., the determination of the size of the smallest scales, is based on the concept of isotropic turbulence. A field $u(t, x)$ is called *statistically stationary* if all statistics of $u(t, x)$ are invariant under a shift of time. It is called *statistically homogeneous* if all statistics are invariant under a shift of position. If the field is also statistically invariant under rotations and reflections of the coordinate system, it is called (*statistically*) *isotropic*. Wind tunnel experiments have been performed on (approximately) isotropic turbulence. However, isotropic turbulence is in general an idealization.

Let $\Omega \subset \mathbb{R}^3$. Richardson [49] gave a description of the physical mechanisms which work in turbulent flows. Large eddies are unstable and break up into smaller ones. Thereby energy is transferred to the smaller eddies. These eddies undergo a similar process. This process is continued until the Reynolds number $\text{Re}(l) = u(l)l/\nu$ of the eddies of size l is sufficiently small (of order one) so that the eddy motion is stable and molecular viscosity is effective in dissipating the kinetic energy. This process is called the energy cascade.

Denote by ε [m^2/s^3] the rate of dissipation of turbulent energy which is defined in the following way. Consider \mathbf{u} as a random variable and let $\langle \mathbf{u} \rangle$ be the mean value (expectation) of \mathbf{u} . The difference $\mathbf{u}' := \mathbf{u} - \langle \mathbf{u} \rangle$ is called the fluctuation. The rate of dissipation of turbulence energy is now defined by

$$\varepsilon := 2\nu \langle \mathbb{D}(\mathbf{u}') : \mathbb{D}(\mathbf{u}') \rangle.$$

The detailed theoretical and experimental study of particular flows shows that

$$(2) \quad \varepsilon \sim \frac{U^3}{L}$$

independently of Re .

In a fundamental paper, Kolmogorov [37] postulated three hypotheses about turbulent flows:

- 1) At sufficiently high Reynolds numbers, the small scale turbulent motions are isotropic.
- 2) In every turbulent flow at sufficiently high Reynolds number, the statistics of the small scale motions have a universal form which is uniquely given by ν and ε .

- 3) In every turbulent flow at sufficiently high Reynolds number, the statistics of motions of scale l in the range $L \gg l \gg \lambda$ have a universal form uniquely determined by ε and independent of ν .

For describing the size of the smallest scales, the first and second hypotheses are of importance.

Let ε and ν be given. Then there are unique length, velocity and time scales which can be defined, the so-called Kolmogorov scales

$$(3) \quad \lambda = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \text{ [m]}, \quad u_\lambda = (\varepsilon\nu)^{1/4} \text{ [m/s]}, \quad t_\lambda = \left(\frac{\nu}{\varepsilon}\right)^{1/2} \text{ [s]}.$$

The Reynolds number of the eddies of size λ is

$$(4) \quad \text{Re}(\lambda) = \frac{\lambda u_\lambda}{\nu} = 1,$$

so that it is sufficiently small for the dissipation to be effective. In addition, using (3), the rate of dissipation is given by

$$(5) \quad \varepsilon = \nu \frac{u_\lambda^2}{\lambda^2} = \nu \frac{1}{t_\lambda^2}.$$

Hence

$$(6) \quad \frac{u_\lambda}{\lambda} = \frac{1}{t_\lambda}.$$

The left-hand side is an approximation to the spatial derivative of the characteristic velocity, which describes the change of the velocity gradient, since λ is small. For the large eddies in turbulent flows, the velocity gradient increases with the Reynolds number since the flow field varies rapidly in space and time. The last equation shows that for the Kolmogorov scales, the velocity gradient is bounded uniformly with respect to the Reynolds number. Hence, (4) and (6) characterize the Kolmogorov scales as dissipative scales.

Now, we can estimate the size of the Kolmogorov scales. Using (2) and (3) gives

$$(7) \quad \frac{\lambda}{L} \sim \left(\frac{\nu^3}{L^3 U^3}\right)^{1/4} = \text{Re}^{-3/4} \iff \lambda \sim \text{Re}^{-3/4}.$$

2.3. The impact of the size of the Kolmogorov scales on numerical simulations

A standard discretization of the Navier-Stokes equations (1), like the Galerkin finite element method (FEM), seeks to simulate the behavior of all scales, including

the Kolmogorov scales. Consider as an example the domain $\Omega = (0, 1)^3$ such that $L = 1$, and a mesh of roughly 10^7 cubic mesh cells ($\approx 215^3$). Assuming that the mesh width is equal to the resolution of the discretization, as for low order finite elements, then $\lambda \approx 1/215$ since smaller scales cannot be represented on the given mesh. Assuming additionally that equality holds in (2), it follows from (7) that flows up to a Reynolds number of $\text{Re} = 215^{4/3} \approx 1290$ can be simulated. This is far less than the Reynolds number of turbulent flows in applications. Thus, numerical simulation of a turbulent flow which is based directly on the Navier-Stokes equations, the so-called Direct Numerical Simulation (DNS), is not feasible.

The small scales are important in the physics of turbulent flows. A numerical scheme which simply neglects them, e.g., by introducing sufficient artificial viscosity, computes a solution which is laminar and lacks important properties of the turbulent solution, e.g., the mean velocity profiles of turbulent channel flows look considerably different from the mean velocity profile of a laminar channel flow. Such a solution is in general useless in applications. The way to treat the small scales which cannot be resolved, consists in modeling their influence onto the resolved scales. In other words, a turbulence model has to be applied.

There are various approaches to turbulence modeling which all have a number of variants, e.g.:

- Reynolds averaged Navier-Stokes equations (RANS),
- turbulent viscosity models, e.g., the famous $k - \varepsilon$ model [45],
- Lagrangian averaged Navier-Stokes equations (LANS),
- large eddy simulation (LES),
- variational multiscale models (VMS or VMS-LES).

In this paper, LES and VMS models will be considered in more detail.

Remark 2.1 (The smallest scales in two-dimensional flows). The smallest scales in two-dimensional flows behave differently from (7). Kraichnan [38] showed that in two dimensions $\lambda = \mathcal{O}(\text{Re}^{-1/2})$.

Remark 2.2 (Vortex stretching—a fundamental difference between two- and three-dimensional flows at high Reynolds number). The vorticity is defined by $\boldsymbol{\omega} = \nabla \times \mathbf{u}$. Applying the curl operator to the Navier-Stokes equations (1) with $\mathbf{f} = \mathbf{0}$ results in the following equation for the vorticity:

$$\frac{\partial \boldsymbol{\omega}}{\partial t} - \text{Re}^{-1} \nabla \cdot \mathbb{D}(\boldsymbol{\omega}) + (\mathbf{u} \cdot \nabla) \boldsymbol{\omega} - (\boldsymbol{\omega} \cdot \nabla) \mathbf{u} = 0.$$

The viscous term is small for high Reynolds numbers and can be neglected. Thus

$$(8) \quad \frac{D\boldsymbol{\omega}}{Dt} = \frac{\partial \boldsymbol{\omega}}{\partial t} + (\mathbf{u} \cdot \nabla) \boldsymbol{\omega} \approx \boldsymbol{\omega} \cdot \nabla \mathbf{u}.$$

This is the equation of an infinitesimal line element of material. If $\nabla \mathbf{u}$ acts so as to stretch the line element then $|\boldsymbol{\omega}|$ will be stretched, too. Thus, in turbulent three-dimensional flows, vortex stretching occurs and this is an important feature of such flows.

In two-dimensional flows, the right-hand side of (8) vanishes. Thus, vortex stretching cannot occur. Because of the absence of this mechanism, two-dimensional flows at high Reynolds numbers are qualitatively different from three-dimensional turbulent flows.

For this reason, one can share the point of view that in two dimensions there are no turbulent flows. However, from the point of view of numerical mathematics it is legitimate to check new methods for high Reynolds number flows also for two-dimensional problems. If they fail, their success for three-dimensional flows, which possess additional complicated features, is very unlikely. On the other hand, if they are successful, it cannot be concluded without numerical studies that they will work well in three dimensions, too.

Suggested readings for more details on the topics in this section are the monographs of Pope [48] and Davidson [8].

3. CLASSICAL LARGE EDDY SIMULATION (LES)

In this paper, standard notations for Lebesgue and Sobolev spaces are used, e.g., see [1]. Spaces of vector-valued functions are denoted with the same symbol as the corresponding space of scalar functions. The inner product in the Lebesgue space $L^2(\Omega)$ is denoted by

$$(u, v) = \int_{\Omega} u(\mathbf{x})v(\mathbf{x}) \, d\mathbf{x}.$$

The Euclidean norm of a vector is denoted by $\|\cdot\|_2$ and the Frobenius norm of a matrix $A \in \mathbb{R}^{n \times n}$ is given by

$$\|A\|_F = (A : A)^{1/2} = \left(\sum_{i,j=1}^n a_{ij}^2 \right)^{1/2}.$$

3.1. The basic approach

The basic idea of (classical) LES consists in defining large scales by averaging in space. This is done by convolution with an appropriate filter function g . The usual way of defining filters in LES for domains in \mathbb{R}^d , $d > 1$, consists in using a tensor product of one-dimensional filters.

Assume that $\Omega = \mathbb{R}^d$, $d \in \{2, 3\}$. The classical LES defines the large scale velocity field and pressure $(\bar{\mathbf{u}}, \bar{p})$ by

$$(9) \quad \bar{\mathbf{u}}(\mathbf{y}) = \frac{1}{\delta(\mathbf{y})^d} \int_{\mathbb{R}^d} g\left(\frac{\mathbf{y} - \mathbf{x}}{\delta(\mathbf{y})}\right) \mathbf{u}(\mathbf{x}) \, d\mathbf{x}, \quad \bar{p}(\mathbf{y}) = \frac{1}{\delta(\mathbf{y})^d} \int_{\mathbb{R}^d} g\left(\frac{\mathbf{y} - \mathbf{x}}{\delta(\mathbf{y})}\right) p(\mathbf{x}) \, d\mathbf{x}.$$

The parameter $\delta(\mathbf{y})$ is the filter width which describes what are the large eddies—these are all eddies of size at least $\delta(\mathbf{y})$. The filter width might be also chosen differently in different directions, like in (23), however, this results in a more complicated general expressions for $(\bar{\mathbf{u}}, \bar{p})$ than (9). The small scales or fluctuations (\mathbf{u}', p') are defined by

$$(10) \quad \mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}}, \quad p' = p - \bar{p}.$$

The task of the filter function is to filter out the small scales or, equivalently, to damp out the high wave number components. LES has the goal to simulate the behavior of $(\bar{\mathbf{u}}, \bar{p})$ accurately.

The simulation of $(\bar{\mathbf{u}}, \bar{p})$ requires equations for these functions. These equations have to be based on the Navier-Stokes equations (1). The usual approach to obtain such equations in the (engineering) literature consists of three steps, e.g., see Sagaut [51]:

- 1) Average the Navier-Stokes equations, i.e., the Navier-Stokes equations are convolved with the filter function. This gives, since convolution is a linear operator,

$$\begin{aligned} \frac{\partial \bar{\mathbf{u}}}{\partial t} - 2\text{Re}^{-1} \overline{\nabla \cdot \mathbb{D}(\mathbf{u})} + \overline{\nabla \cdot (\mathbf{u}\mathbf{u}^T)} + \overline{\nabla p} &= \bar{\mathbf{f}} \quad \text{in } (0, T] \times \mathbb{R}^d, \\ \overline{\nabla \cdot \mathbf{u}} &= 0 \quad \text{in } (0, T] \times \mathbb{R}^d, \\ \bar{\mathbf{u}}(0, \cdot) &= \bar{\mathbf{u}}_0 \quad \text{in } \mathbb{R}^d. \end{aligned}$$

Here, the identity $(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot (\mathbf{u}\mathbf{u}^T)$ has been used.

- 2) Now, it is assumed that one can simply interchange the convolution operator and all differentiation operators. This results in the so-called space averaged Navier-Stokes equations

$$(11) \quad \begin{aligned} \frac{\partial \bar{\mathbf{u}}}{\partial t} - 2\text{Re}^{-1} \nabla \cdot \mathbb{D}(\bar{\mathbf{u}}) + \nabla \cdot (\bar{\mathbf{u}} \bar{\mathbf{u}}^T) + \nabla \cdot \mathcal{R}(\mathbf{u}, \mathbf{u}) + \nabla \bar{p} &= \bar{\mathbf{f}} \quad \text{in } (0, T] \times \mathbb{R}^d, \\ \nabla \cdot \bar{\mathbf{u}} &= 0 \quad \text{in } (0, T] \times \mathbb{R}^d, \\ \bar{\mathbf{u}}(0, \cdot) &= \bar{\mathbf{u}}_0 \quad \text{in } \mathbb{R}^d \end{aligned}$$

with the Reynolds stress tensor

$$(12) \quad \mathcal{R}(\mathbf{u}, \mathbf{u}) = \overline{\mathbf{u} \mathbf{u}^T} - \bar{\mathbf{u}} \bar{\mathbf{u}}^T.$$

The assumption in this step is valid for the partial derivative with respect to time. With respect to the spatial derivatives, it is valid only in special cases, e.g., if $\Omega = \mathbb{R}^d$. This assumption is wrong in general. A so-called commutation error will be committed if (11) is used in such situations. Commutation errors will be studied in more detail in Section 3.2.

- 3) Using the decomposition (10) and the linearity of the convolution, the Reynolds stress tensor can be written in the form

$$(13) \quad \mathcal{R}(\mathbf{u}, \mathbf{u}) = \overline{\bar{\mathbf{u}} \bar{\mathbf{u}}^T} + \overline{\bar{\mathbf{u}} \mathbf{u}'^T} + \overline{\mathbf{u}' \bar{\mathbf{u}}^T} + \overline{\mathbf{u}' \mathbf{u}'^T} - \bar{\mathbf{u}} \bar{\mathbf{u}}^T.$$

At this point, a model of the influence of the small scales \mathbf{u}' onto the large scales $(\bar{\mathbf{u}}, \bar{p})$ is needed since there is no mathematical way to get rid of \mathbf{u}' . The development of appropriate models is the main issue in LES. This topic will be addressed in Section 3.3.

3.2. Commutation errors

In the study of the commutation of convolution and spatial differentiation operators, one has to distinguish two situations. The former is that the filter g possesses unbounded support and the latter is the case of g having compact support. Both cases have been addressed in literature.

The presence of commutation errors in the derivation of the space averaged Navier-Stokes equations has been known for a long time. It was (and by many people still is) believed that these errors are negligible or of higher order. In practice, they are simply ignored. However, new analytical results and numerical studies show that there are commutation errors, in particular, near the boundary of a bounded domain Ω , which are of great importance.

3.2.1. Filters with unbounded support. The most popular filter with this property is the Gaussian filter

$$(14) \quad g_\delta(\mathbf{x}) = \left(\frac{\gamma}{\delta^2 \pi}\right)^{d/2} \exp\left(-\frac{\gamma}{\delta^2} \|\mathbf{x}\|_2^2\right)$$

with $\gamma = 6$, see Fig. 1. In this section, $\delta > 0$ is assumed to be a constant.

The application of the Gaussian filter to the Navier-Stokes equations in the first step of the general approach requires that all functions are defined in \mathbb{R}^d so that the integrals in (9) are well defined. We will study the commutation error in the case that $\Omega \subset \mathbb{R}^d$ is a bounded domain. This is the most common situation in applications. The Navier-Stokes equations will be equipped with homogeneous Dirichlet boundary conditions $\mathbf{u} = \mathbf{0}$ on $\partial\Omega$. In addition, we assume that $\partial\Omega$ is a Lipschitz boundary. In

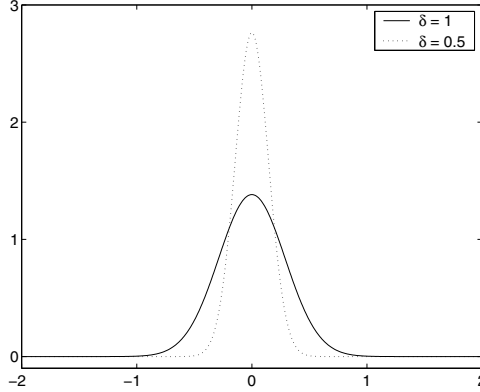


Figure 1. The Gaussian filter in one dimension for different δ , $\gamma = 6$.

particular, $\partial\Omega$ has a finite $(d - 1)$ -dimensional measure. The solution of the Navier-Stokes equations (1) is assumed to exist uniquely and to possess the regularity

$$\begin{aligned} \mathbf{u} \in H^2(\Omega) \cap H_0^1(\Omega), \quad p \in H^1(\Omega) \cap L_0^2(\Omega) \quad \text{for a.e. } t \in [0, T], \\ \mathbf{u} \in H^1((0, T)) \quad \text{for a.e. } \mathbf{x} \in \overline{\Omega}. \end{aligned}$$

The regularity with respect to time is not of importance for the commutation error since LES uses spatial averaging and not time averaging. The regularity with respect to space is a standard assumption for the steady state Navier-Stokes equations.

Before the Navier-Stokes equations can be convolved, all functions have to be extended off Ω so that two requirements are fulfilled:

- the extensions have to be computable, since they are needed to compute $(\bar{\mathbf{u}}, \bar{p})$ also in Ω ,
- the extended functions should satisfy the Navier-Stokes equations.

Because of the homogeneous Dirichlet boundary conditions, the trivial extension $\mathbf{u} \equiv \mathbf{0}$ in $\mathbb{R}^d \setminus \Omega$ is natural. Also the pressure p will be extended trivially. The regularity of the extended functions is as follows:

$$(15) \quad \begin{aligned} \mathbf{u} \in H_0^1(\mathbb{R}^d), \quad p \in L_0^2(\mathbb{R}^d) \quad \text{for a.e. } t \in [0, T], \\ \mathbf{u} \in H^1((0, T)) \quad \text{for a.e. } \mathbf{x} \in \mathbb{R}^d. \end{aligned}$$

Now, \mathbf{f} has to be extended so that the second requirement is fulfilled. The insertion of the extended velocity and pressure into the left-hand side of the Navier-Stokes equations requires to define $\nabla \cdot \mathbb{D}(\mathbf{u})$ and ∇p in the sense of distributions. Let

$\varphi \in C_0^\infty(\mathbb{R}^d)$. Since $p \equiv 0$ on $\mathbb{R}^d \setminus \Omega$ for all times, we get

$$(16) \quad (\nabla p)(\varphi)(t) := - \int_{\mathbb{R}^d} p(t, \mathbf{x}) \nabla \varphi(\mathbf{x}) \, d\mathbf{x} \\ = \int_{\Omega} \varphi(\mathbf{x}) \nabla p(t, \mathbf{x}) \, d\mathbf{x} - \int_{\partial\Omega} \varphi(\mathbf{s}) p(t, \mathbf{s}) \mathbf{n}_{\partial\Omega}(\mathbf{s}) \, d\mathbf{s}.$$

In the same way, one obtains

$$(17) \quad \nabla \cdot \mathbb{D}(\mathbf{u})(\varphi)(t) := - \int_{\mathbb{R}^d} \mathbb{D}(\mathbf{u})(t, \mathbf{x}) \nabla \varphi(\mathbf{x}) \, d\mathbf{x} \\ = \int_{\Omega} \varphi(\mathbf{x}) \nabla \cdot \mathbb{D}(\mathbf{u})(t, \mathbf{x}) \, d\mathbf{x} - \int_{\partial\Omega} \varphi(\mathbf{s}) \mathbb{D}(\mathbf{u})(t, \mathbf{s}) \mathbf{n}_{\partial\Omega}(\mathbf{s}) \, d\mathbf{s}.$$

Both distributions have compact support. From (16) and (17), it follows that the extended functions (\mathbf{u}, p) fulfil the distributional form of the momentum equation

$$(18) \quad (\mathbf{u}_t - 2\text{Re}^{-1} \nabla \cdot \mathbb{D}(\mathbf{u}) + \nabla \cdot (\mathbf{u}\mathbf{u}^T) + \nabla p)(\varphi)(t) \\ = \mathbf{f}(\varphi)(t) + \int_{\partial\Omega} \mathbb{S}(\mathbf{u}, p)(t, \mathbf{s}) \mathbf{n}_{\partial\Omega}(\mathbf{s}) \varphi(\mathbf{s}) \, d\mathbf{s},$$

where

$$\mathbb{S}(\mathbf{u}, p) = 2\text{Re}^{-1} \mathbb{D}(\mathbf{u}) - p\mathbb{I}$$

is the stress tensor.

Equation (18) can be convolved and convolution and differentiation commute, [22], [50]. One obtains the space averaged momentum equation

$$\bar{\mathbf{u}}_t - 2\text{Re}^{-1} \nabla \cdot \mathbb{D}(\bar{\mathbf{u}}) + \nabla \cdot (\overline{\mathbf{u}\mathbf{u}^T}) + \nabla \bar{p} \\ = \bar{\mathbf{f}} + \int_{\partial\Omega} g(\mathbf{x} - \mathbf{s}) \mathbb{S}(\mathbf{u}, p)(t, \mathbf{s}) \mathbf{n}_{\partial\Omega}(\mathbf{s}) \, d\mathbf{s} \quad \text{in } (0, T] \times \mathbb{R}^d,$$

for details of the derivation see [9], [29]. In contrast to the naive approach which leads to (11), there is the additional term

$$(19) \quad \int_{\partial\Omega} g(\mathbf{x} - \mathbf{s}) \mathbb{S}(\mathbf{u}, p)(t, \mathbf{s}) \mathbf{n}_{\partial\Omega}(\mathbf{s}) \, d\mathbf{s}$$

on the right-hand side of the momentum equation. This term describes exactly the commutation error. There is no commutation error in the mass equation. The quantity $\mathbb{S}(\mathbf{u}, p)(t, \mathbf{s}) \mathbf{n}_{\partial\Omega}(\mathbf{s})$ is the normal stress on the boundary. From the regularity assumptions (15) on (\mathbf{u}, p) , we have that for almost every $t \in [0, T]$,

$$\mathbb{S}(\mathbf{u}, p) \mathbf{n}_{\partial\Omega} \in L^q(\partial\Omega)$$

with $1 \leq q < \infty$ if $d = 2$ and $1 \leq q \leq 4$ if $d = 3$, e.g., see [14].

The regularity of the commutation error (19) makes the study of expressions of the form

$$(20) \quad \int_{\partial\Omega} g_\delta(\mathbf{x} - \mathbf{s})\psi(\mathbf{s}) \, ds$$

with $\psi \in L^q(\partial\Omega)$, $1 \leq q \leq \infty$, necessary. It can be shown that (20) belongs to $L^p(\mathbb{R}^d)$, $1 \leq p \leq \infty$, see [9], [29]. One important result about the asymptotic behavior of (20) is the following theorem.

Theorem 3.1. *Let $\psi \in L^p(\partial\Omega)$, $1 \leq p \leq \infty$. A necessary and sufficient condition for*

$$(21) \quad \lim_{\delta \rightarrow 0} \left\| \int_{\partial\Omega} g_\delta(\mathbf{x} - \mathbf{s})\psi(\mathbf{s}) \, ds \right\|_{L^p(\mathbb{R}^d)} = 0,$$

$1 \leq p \leq \infty$, is that ψ vanishes almost everywhere on $\partial\Omega$.

Proof. It is obvious that the condition is sufficient.

Let (21) hold and let $p^{-1} + q^{-1} = 1$. From Hölder's inequality, we obtain for an arbitrary function $\varphi \in C_0^\infty(\mathbb{R}^d)$

$$(22) \quad \lim_{\delta \rightarrow 0} \left| \int_{\mathbb{R}^d} \varphi(\mathbf{x}) \left(\int_{\partial\Omega} g_\delta(\mathbf{x} - \mathbf{s})\psi(\mathbf{s}) \, ds \right) \, d\mathbf{x} \right| \\ \leq \lim_{\delta \rightarrow 0} \|\varphi\|_{L^q(\mathbb{R}^d)} \left\| \int_{\partial\Omega} g_\delta(\mathbf{x} - \mathbf{s})\psi(\mathbf{s}) \, ds \right\|_{L^p(\mathbb{R}^d)} = 0.$$

By Fubini's theorem, the symmetry of the Gaussian filter, $g(\mathbf{x}) = g(-\mathbf{x})$, and a well known property of limits of convolutions, e.g., see Folland [13, Theorem 0.13], we have

$$\lim_{\delta \rightarrow 0} \int_{\mathbb{R}^d} \varphi(\mathbf{x}) \left(\int_{\partial\Omega} g_\delta(\mathbf{x} - \mathbf{s})\psi(\mathbf{s}) \, ds \right) \, d\mathbf{x} = \lim_{\delta \rightarrow 0} \int_{\partial\Omega} \psi(\mathbf{s}) \left(\int_{\mathbb{R}^d} g_\delta(\mathbf{x} - \mathbf{s})\varphi(\mathbf{x}) \, d\mathbf{x} \right) \, ds \\ = \int_{\partial\Omega} \psi(\mathbf{s})\varphi(\mathbf{s}) \, ds.$$

From (22) it follows now that

$$0 = \left| \int_{\partial\Omega} \psi(\mathbf{s})\varphi(\mathbf{s}) \, ds \right|$$

for every $\varphi \in C_0^\infty(\mathbb{R}^d)$. This is true if and only if ψ vanishes almost everywhere on $\partial\Omega$. □

The statement of the theorem tells us that the commutation error vanishes in $L^p(\mathbb{R}^d)$ if and only if the normal stress on the boundary is zero for all times. This is exactly the case if there is no interaction between the turbulent flow and the boundary. This situation is very unlikely in applications! Another consequence concerns discretizations which are based on the strong formulation of the underlying equation, like finite difference methods. For such discretizations, the effect of neglecting a term in the equation can be measured in the norm of a Lebesgue space. Thus, for such discretizations, it cannot be expected that the commutation error (19) vanishes as $\delta \rightarrow 0$.

Other discretizations, like finite element methods, are based on a weak or variational formulation of the underlying equation. The effect of neglecting a term of the weak formulation can be measured in a weaker norm, e.g., in the $H^{-1}(\Omega)$ norm. It is shown in [9], [29] that the commutation error (20) tends to zero in $H^{-1}(\Omega)$ as $\delta \rightarrow 0$ with the order of convergence of $1/2$. This order is probably not optimal.

3.2.2. Filters with compact support. The most popular filter in this class is the box filter given in its normalized form by

$$g(x) = \begin{cases} 1 & x \in [-1/2, 1/2], \\ 0 & \text{else.} \end{cases}$$

With this filter, the space averaged velocity is defined by

$$(23) \quad \bar{\mathbf{u}}(\mathbf{y}) = \frac{1}{8\delta_1(\mathbf{y})\delta_2(\mathbf{y})\delta_3(\mathbf{y})} \int_{y_1-\delta_1(\mathbf{y})}^{y_1+\delta_1(\mathbf{y})} \int_{y_2-\delta_2(\mathbf{y})}^{y_2+\delta_2(\mathbf{y})} \int_{y_3-\delta_3(\mathbf{y})}^{y_3+\delta_3(\mathbf{y})} \mathbf{u}(\mathbf{x}) \, d\mathbf{x}.$$

The appealing advantage of this type of filter is that the filter widths in the different directions $\delta_1(\mathbf{y})$, $\delta_2(\mathbf{y})$, $\delta_3(\mathbf{y})$ can be chosen such that the domain of integration is always contained in $\bar{\Omega}$. However, approaching the boundary, the filter width has to tend to zero, at least in one direction. Thus, the filter width is not constant and for this reason a commutation error arises.

The commutation error due to a non-constant filter width in the box filter can be studied already in one dimension, [3]. Straightforward calculations give the following formula for the commutation error in this case:

$$(24) \quad \mathcal{E}_c(y) := \frac{d}{dy} \bar{u}(y) - \overline{\frac{du}{dy}}(y) \\ = \frac{\delta'(y)}{\delta(y)} \left(\frac{1}{2\delta(y)} \int_{y-\delta(y)}^{y+\delta(y)} x u'(x) \, dx - \frac{y}{2\delta(y)} \int_{y-\delta(y)}^{y+\delta(y)} u'(x) \, dx \right).$$

The evaluation of this error requires the knowledge of u , which stands for one component of the velocity or for the pressure. However, in turbulent flows, an analytical expression for the solution of the Navier-Stokes equations is not available.

The commutation error is of interest in particular at the boundary. There are empirical laws of the average form of the boundary layer which can be substituted into (24) providing in this way information on the average commutation error. Consider, e.g., the $1/\alpha$ th power law

$$u(y) = \begin{cases} U_\infty \left(\frac{y}{\eta}\right)^{1/\alpha}, & 0 \leq y \leq \eta, \\ U_\infty, & \eta < y, \end{cases}$$

where U_∞ is the free stream velocity, $\alpha > 1$ and η is the boundary layer thickness, see [52]. Often, $\alpha = 7$ is used.

We are interested in the behavior inside the boundary layer, i.e. $0 < y < \eta$. Approaching the boundary, it is required that the filter width tends to zero. The choice $\delta(y) = \mathcal{O}(y^q)$, $q \geq 1$, satisfies this condition. Then, the commutation error (24) can be evaluated and a series expansion leads to the estimate

$$|\mathcal{E}_c(y)| \leq C y^{2q+1/\alpha-3}$$

for y sufficiently close to the boundary. Thus, the requirement for the convergence of the commutation error in a neighborhood of the boundary is $q > \frac{1}{2}(3 - 1/\alpha)$. Numerical tests, [3], show that this estimate is sharp.

The convergence of the commutation error in the case that the mean flow obeys the $1/\alpha$ th power law at the wall is only guaranteed if the filter width tends to zero sufficiently fast near the boundary. Since in computations the filter width has to be larger than the mesh width, this implies that the mesh has to be very fine at the wall. In practice, the convergence of the commutation error requires that the boundary layer must be resolved in the numerical simulation.

A similar result is obtained if the flow has singularities at the boundary, e.g., at a reentrant corner. Also in this situation, convergence of the commutation error requires that the filter width $\delta(y)$ must be sufficiently small near the singularity so that in practice a resolution of the flow field at the singularity becomes necessary.

In LES modeling, the question arises of what is more important: to model the Reynolds stress tensor (12) or the commutation error. In this comparison, one has to consider the divergence of the Reynolds stress tensor since this term has to be modeled in the space averaged Navier-Stokes equations (11). This question was investigated in [55] while the focus of this paper is on turbulent flows which are well separated from solid bounding walls. Assuming existence and convergence of the

Taylor series expansion of the velocity \mathbf{u} , it is shown that for n th order filters (the first non-vanishing moment of the filter function is the n th moment) the commutation error and the divergence of the Reynolds stress tensor are asymptotically of the same order. Numerical studies of a turbulent mixing layer flow show, however, that for the box filter (second order filter) the contribution of the divergence of the Reynolds stress tensor is by one order of magnitude larger than the contribution of the commutation error if the filter width varies slowly. This indicates that the pre-factors of the leading order term in the expansion of the commutation error and the divergence of the Reynolds stress tensor are of considerably different sizes. A sharp variation of the filter width increases the size of the commutation error considerably. It is concluded that in this case a modeling of this error should be done. Two models for the commutation error are proposed in [55] and tested on a turbulent mixing layer flow.

In [5], the asymptotic behavior of commutation errors, originating from the application of the non-uniform box filter, and the divergence of the Reynolds stress tensor are studied at solid boundaries for the turbulent channel flow. In the analysis, the unknown flow field is modeled by a couple of wall laws (Reichardt law and $1/\alpha$ th power law) for the mean velocity profile, and highly oscillating functions model the turbulent fluctuations. The asymptotics which are derived show that near the wall, the commutation errors are at least as important as the divergence of the Reynolds stress tensor.

3.3. Modeling the Reynolds stress tensor

The modeling of the Reynolds stress tensor $\mathcal{R}(\mathbf{u}, \mathbf{u})$ given in (12) is the main issue in classical LES.

3.3.1. Eddy viscosity models. The simplest form of an eddy viscosity model is

$$(25) \quad \mathcal{R}(\mathbf{u}, \mathbf{u}) - \frac{\text{tr}(\mathcal{R}(\mathbf{u}, \mathbf{u}))}{3} \mathbb{1} = -\nu_T \mathbb{D}(\bar{\mathbf{u}}),$$

where ν_T is called the turbulent viscosity and $\text{tr}(\mathcal{R}(\mathbf{u}, \mathbf{u}))$ is the trace of $\mathcal{R}(\mathbf{u}, \mathbf{u})$. Model (25) is called the Reynolds closure or Boussinesq hypothesis, see, e.g., [45].

The second term on the left-hand side is usually added to the pressure, defining a new pressure, which is for simplicity of notation also denoted by \bar{p} ,

$$\bar{p} := \bar{p} + \frac{\text{tr}(\mathcal{R}(\mathbf{u}, \mathbf{u}))}{3}.$$

The simplest LES model which is based on (25) is the Smagorinsky model. Let L_{int} be the so-called integral length scale of the eddies containing energy (the large

eddies) and U_{int} the corresponding characteristic velocity. From (2) it follows that

$$(26) \quad \varepsilon \sim \frac{U_{\text{int}}^3}{L_{\text{int}}}.$$

The smallest resolved scales, which are of size δ , are still much larger than the Kolmogorov scales. Thus, the filter width δ and the corresponding velocity U_δ of these scales can be also used as characteristic length and velocity, respectively. Hence, we have

$$(27) \quad \varepsilon \sim \frac{U_\delta^3}{\delta}.$$

From (26) and (27) it follows that

$$(28) \quad U_\delta \sim U_{\text{int}} \left(\frac{\delta}{L_{\text{int}}} \right)^{1/3}.$$

The eddy viscosity model captures the dissipation of the eddies of size δ . Similarly to the derivation of (5) for the Kolmogorov scales, one obtains

$$(29) \quad \varepsilon \sim \nu_T \frac{U_\delta^2}{\delta^2}.$$

Inserting (27) and (28) into (29) gives

$$\nu_T \sim U_\delta \delta \sim U_{\text{int}} L_{\text{int}}^{-1/3} \delta^{4/3}.$$

Now, the assumption

$$U_{\text{int}} \sim L_{\text{int}} \|\mathbb{D}(\bar{\mathbf{u}})\|_F$$

is used. One gets, by replacing the similarity sign with a factor,

$$\nu_T = c L_{\text{int}}^{2/3} \delta^{4/3} \|\mathbb{D}(\bar{\mathbf{u}})\|_F.$$

The integral length scale L_{int} is hard to determine. For this reason, one uses the approximation $L_{\text{int}} \sim \delta$ and gets finally the Smagorinsky model

$$(30) \quad \nu_T = c_S \delta^2 \|\mathbb{D}(\bar{\mathbf{u}})\|_F,$$

where c_S is a user-chosen constant. The Smagorinsky model is quite popular because of its simplicity. However, it has some well known drawbacks and computes often inaccurate results, e.g., see [57], [51]. The great difficulty in the application of the Smagorinsky model consists in a good choice of the constant c_S . It is even very

likely that one has to choose different constants in different flow regions and at different times to obtain good simulations. Note the Smagorinsky model does in general not vanish in situation where a turbulence model is not needed, e.g., for laminar flows. Generally, numerical simulations with the Smagorinsky model lead to over-diffusive results. From the mathematical point of view, the Smagorinsky model is well understood. Ladyzhenskaya [39] could prove the existence and uniqueness of an appropriately defined weak solution in two and three dimensions applying the Galerkin method. The main analytical tool is the proof of monotonicity of the non-linear viscous term which is introduced by the Smagorinsky model. The analysis of the Smagorinsky model with variable but positive $c_S(t, \mathbf{x})$ can be found in Świerczewska [54]. In [34], one can find finite element error estimates for the Smagorinsky model.

The most popular variant of the Smagorinsky model is the dynamic subgrid scale (SGS) model by Germano et al. [17] and Lilly [44]. In this model, c_S is a function in space and time, $c_S = c_S(t, \mathbf{x})$, which is computed a posteriori.

The dynamic subgrid scale model starts with introducing a second filter, the so-called test filter denoted by an arrow, with $\overleftarrow{\delta} > \delta$. Then, the space averaged Navier-Stokes equations (11) are filtered once more with the test filter. Assuming that differentiation and filtering commute yields

$$\begin{aligned} \overleftarrow{\mathbf{u}}_t - 2\text{Re}^{-1}\nabla \cdot \mathbb{D}(\overleftarrow{\mathbf{u}}) + \nabla \cdot (\overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T) + \nabla \cdot \overleftarrow{\mathcal{R}}(\mathbf{u}, \mathbf{u}) + \nabla \overleftarrow{p} &= \overleftarrow{\mathbf{f}} \quad \text{in } (0, T] \times \Omega, \\ \nabla \cdot \overleftarrow{\mathbf{u}} &= 0 \quad \text{in } [0, T] \times \Omega. \end{aligned}$$

A direct calculation gives

$$(31) \quad \mathcal{K} - \overleftarrow{\mathcal{R}}(\mathbf{u}, \mathbf{u}) = \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T - \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T$$

with $\mathcal{K} = \overleftrightarrow{\mathbf{u}} \overleftrightarrow{\mathbf{u}}^T - \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T$. Inserting the ansatz

$$\begin{aligned} \mathcal{R}(\mathbf{u}, \mathbf{u})(t, \mathbf{x}) - \frac{\text{tr}(\mathcal{R}(\mathbf{u}, \mathbf{u}))}{3} \mathbb{1} &= -c_S(t, \mathbf{x}) \delta^2 \|\mathbb{D}(\bar{\mathbf{u}})\|_F \mathbb{D}(\bar{\mathbf{u}}), \\ \mathcal{K}(t, \mathbf{x}) - \frac{\text{tr}(\mathcal{K})}{3} \mathbb{1} &= -c_S(t, \mathbf{x}) \overleftarrow{\delta}^2 \|\mathbb{D}(\overleftarrow{\mathbf{u}})\|_F \mathbb{D}(\overleftarrow{\mathbf{u}}) \end{aligned}$$

into (31), one obtains

$$(32) \quad \begin{aligned} \mathbf{0} &= -\overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T + \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T + \frac{1}{3} \left(\text{tr}(\mathcal{K}) - \text{tr}(\overleftarrow{\mathcal{R}}(\mathbf{u}, \mathbf{u})) \right) \mathbb{1} \\ &\quad + \overleftarrow{(c_S(t, \mathbf{x}) \delta^2 \|\mathbb{D}(\bar{\mathbf{u}})\|_F \mathbb{D}(\bar{\mathbf{u}}))} - c_S(t, \mathbf{x}) \overleftarrow{\delta}^2 \|\mathbb{D}(\overleftarrow{\mathbf{u}})\|_F \mathbb{D}(\overleftarrow{\mathbf{u}}). \end{aligned}$$

The linearity of the filter, the linearity of the trace operator and (31) yield

$$(33) \quad \text{tr}(\mathcal{K}) - \overleftarrow{\text{tr}(\mathcal{R}(\mathbf{u}, \mathbf{u}))} = \text{tr}\left(\mathcal{K} - \overleftarrow{\mathcal{R}(\mathbf{u}, \mathbf{u})}\right) = \text{tr}\left(\overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T - \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T\right).$$

In order to derive equations for $c_S(t, \mathbf{x})$, the approximation

$$(34) \quad \overleftarrow{(c_S(t, \mathbf{x}) \delta^2 \|\mathcal{D}(\bar{\mathbf{u}})\|_F \mathbb{D}(\bar{\mathbf{u}))}} \approx c_S(t, \mathbf{x}) \delta^2 \overleftarrow{(\|\mathbb{D}(\bar{\mathbf{u}})\|_F \mathbb{D}(\bar{\mathbf{u}))}}$$

is used. If c_S depends only on t but not on \mathbf{x} , one has an equality instead of an approximation. Inserting (34) and (33) into (32) gives

$$(35) \quad \begin{aligned} \mathbf{0} \approx & -\overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T + \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T + \frac{1}{3} \text{tr}\left(\overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T - \overleftarrow{\mathbf{u}} \overleftarrow{\mathbf{u}}^T\right) \mathbb{I} \\ & + c_S(t, \mathbf{x}) \left(\delta^2 \overleftarrow{(\|\mathbb{D}(\bar{\mathbf{u}})\|_F \mathbb{D}(\bar{\mathbf{u}))}} - \overleftarrow{\delta^2 \|\mathbb{D}(\bar{\mathbf{u}})\|_F \mathbb{D}(\bar{\mathbf{u}))}} \right) \\ =: & \mathbb{L} + c_S(t, \mathbf{x}) \mathbb{M}. \end{aligned}$$

Equations for $c_S(t, \mathbf{x})$ are obtained by replacing the approximation sign in (35) with the equal sign. Then, there are $\frac{1}{2}d(d+1)$ equations to determine a single constant for given t and \mathbf{x} . Because of the divergence constraint, the traces of the deformation tensors vanish, so that only $\frac{1}{2}d(d+1) - 1$ equations are linearly independent. Lilly [44] proposed to determine the parameter $c_S(t, \mathbf{x})$ by the least squares method, i.e. to find $c_S(t, \mathbf{x})$ such that $\|\mathbb{L} + c_S(t, \mathbf{x}) \mathbb{M}\|_F^2$ is minimized. A direct calculation gives

$$c_S(t, \mathbf{x}) = \frac{\mathbb{L} : \mathbb{M}}{\mathbb{M} : \mathbb{M}}(t, \mathbf{x}).$$

In practical computations, the test filter can be applied by solving the space averaged Navier-Stokes equations on a coarse grid. In the case of uniformly refined grids, the use of the next grid coarser than the current one results in $\overleftarrow{\delta} = 2\delta$.

The practical use of this approach shows that one has to smooth (average) $c_S(t, \mathbf{x})$ in space and time to obtain stable simulations. Otherwise, large negative values can be computed for $c_S(t, \mathbf{x})$ which lead to a blow up of the simulations. The choice of smoothing strategies is done heuristically and requires a lot of experience. Altogether, the dynamic SGS model is considered currently to be the best performing classical LES model.

3.3.2. Methods which are based on the approximation of the Fourier transform of the filter. Let δ be a positive constant. The starting point of these models is the decomposition (13) of the Reynolds stress tensor. To each term on the right-hand side, save the last one, the following procedure is applied:

1. computing the Fourier transform $\mathcal{F}(\cdot)$,
2. replacing $\mathcal{F}(\mathbf{u}')$ by a function of $\mathcal{F}(\bar{\mathbf{u}})$ if necessary,
3. approximating the Fourier transform of the Gaussian filter by an appropriate simpler function,
4. neglecting all terms which are formally of order δ^4 or higher,
5. computing the inverse Fourier transform.

The crucial step is the third one. There are two proposals in literature concerning this approximation.

The most important task of the filter function, to damp out the high wave number components, will be reflected by the property that the Fourier transform of the filter function (almost) vanishes for high wave numbers, see Figs. 2 and 3 for the Gaussian filter.

The five steps are now considered in detail. A straightforward computation gives for the first step

$$(36) \quad \begin{aligned} \mathcal{F}(\overline{\mathbf{u} \mathbf{u}^T}) &= \mathcal{F}(g_\delta) \mathcal{F}(\bar{\mathbf{u}} \bar{\mathbf{u}}^T), \\ \mathcal{F}(\overline{\mathbf{u} \mathbf{u}'^T}) &= \mathcal{F}(g_\delta) (\mathcal{F}(\bar{\mathbf{u}}) * \mathcal{F}(\mathbf{u}')^T), \\ \mathcal{F}(\overline{\mathbf{u}' \mathbf{u}^T}) &= \mathcal{F}(g_\delta) (\mathcal{F}(\mathbf{u}') * \mathcal{F}(\bar{\mathbf{u}})^T), \\ \mathcal{F}(\overline{\mathbf{u}' \mathbf{u}'^T}) &= \mathcal{F}(g_\delta) (\mathcal{F}(\mathbf{u}') * \mathcal{F}(\mathbf{u}')^T). \end{aligned}$$

To perform the second step, we have to assume that the Fourier transform of the filter is never equal to zero. This is fulfilled, e.g., by the Gaussian filter. Using the decomposition (10), one obtains

$$\mathcal{F}(\mathbf{u}') = \left(\frac{1}{\mathcal{F}(g_\delta)} - 1 \right) \mathcal{F}(\bar{\mathbf{u}}).$$

Inserting this into (36) gives

$$\begin{aligned} \mathcal{F}(\overline{\mathbf{u} \mathbf{u}'^T}) &= \mathcal{F}(g_\delta) \left(\mathcal{F}(\bar{\mathbf{u}}) * \left(\frac{1}{\mathcal{F}(g_\delta)} - 1 \right) \mathcal{F}(\bar{\mathbf{u}})^T \right), \\ \mathcal{F}(\overline{\mathbf{u}' \mathbf{u}^T}) &= \mathcal{F}(g_\delta) \left(\left(\frac{1}{\mathcal{F}(g_\delta)} - 1 \right) \mathcal{F}(\bar{\mathbf{u}}) * \mathcal{F}(\bar{\mathbf{u}})^T \right), \\ \mathcal{F}(\overline{\mathbf{u}' \mathbf{u}'^T}) &= \mathcal{F}(g_\delta) \left(\left(\frac{1}{\mathcal{F}(g_\delta)} - 1 \right) \mathcal{F}(\bar{\mathbf{u}}) * \left(\frac{1}{\mathcal{F}(g_\delta)} - 1 \right) \mathcal{F}(\bar{\mathbf{u}})^T \right). \end{aligned}$$

In the third step, $\mathcal{F}(g_\delta)$ and $1/\mathcal{F}(g_\delta)$ have to be approximated by simpler functions. In [42], [6], [2], the use of a second order Taylor polynomial is proposed, see Fig. 2,

$$\mathcal{F}(g_\delta)(\delta, \mathbf{y}) = 1 - \frac{\|\mathbf{y}\|_2^2}{4\gamma} \delta^2 + \mathcal{O}(\delta^4), \quad \frac{1}{\mathcal{F}(g_\delta)}(\delta, \mathbf{y}) = 1 + \frac{\|\mathbf{y}\|_2^2}{4\gamma} \delta^2 + \mathcal{O}(\delta^4).$$

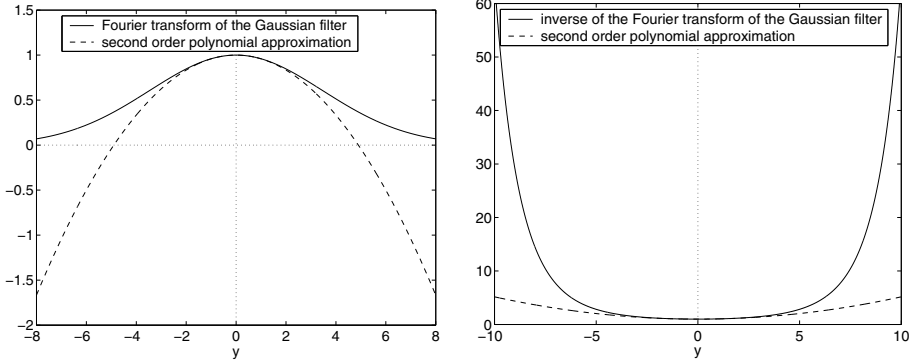


Figure 2. $\mathcal{F}(g_\delta)$ and $1/\mathcal{F}(g_\delta)$ with their polynomial approximations, Gaussian filter with $\gamma = 6$, $\delta = 1$.

The resulting model is called the gradient model or the Taylor LES model. Direct calculations give

$$\begin{aligned}\mathcal{F}(\overline{\mathbf{u} \mathbf{u}^T}) &= \mathcal{F}(\mathbf{u} \mathbf{u}^T) + \frac{\delta^2}{4\gamma} \mathcal{F}(\Delta(\mathbf{u} \mathbf{u}^T)) + \mathcal{O}^{\text{formal}}(\delta^4), \\ \mathcal{F}(\overline{\mathbf{u} \mathbf{u}'^T}) &= -\frac{\delta^2}{4\gamma} \mathcal{F}(\mathbf{u} \Delta(\mathbf{u})^T) + \mathcal{O}^{\text{formal}}(\delta^4), \\ \mathcal{F}(\overline{\mathbf{u}' \mathbf{u}^T}) &= -\frac{\delta^2}{4\gamma} \mathcal{F}(\Delta(\mathbf{u}) \mathbf{u}^T) + \mathcal{O}^{\text{formal}}(\delta^4), \\ \mathcal{F}(\overline{\mathbf{u}' \mathbf{u}'^T}) &= \mathcal{O}^{\text{formal}}(\delta^4).\end{aligned}$$

The notation $\mathcal{O}^{\text{formal}}(\delta^4)$ means that there are expressions of the form δ^4 multiplied with functions which involve \mathbf{u} which in turn depends also on δ .

In the fourth step, all terms which are formally of the fourth order in δ are neglected. Then, the inverse Fourier transform in Step 5 can be performed easily. Collecting terms gives finally

$$(37) \quad \mathcal{R}(\mathbf{u}, \mathbf{u}) \approx \frac{\delta^2}{2\gamma} \nabla \mathbf{u} \nabla \mathbf{u}^T.$$

It can be observed that the polynomial approximation of $\mathcal{F}(g_\delta)$ is a good approximation only for small wave numbers while it is completely wrong for high wave numbers. This means that the most important property of the Gaussian filter function is not preserved by its Taylor polynomial approximation!

Based on this observation, Galdi and Layton [16] proposed to use a rational approximation of the exponential

$$e^{ax} = \frac{1}{1+ax} + \mathcal{O}(a^2 x^2).$$

Applying this subdiagonal Padé approximation to $\mathcal{F}(g_\delta)$ gives

$$(38) \quad \mathcal{F}(g_\delta)(\delta, \mathbf{y}) = \frac{1}{1 + \frac{\|\mathbf{y}\|_2^2}{4\gamma} \delta^2} + \mathcal{O}(\delta^4)$$

and transforming this formula to $1/\mathcal{F}(g_\delta)$ yields

$$(39) \quad \frac{1}{\mathcal{F}(g_\delta)}(\delta, \mathbf{y}) = 1 + \frac{\|\mathbf{y}\|_2^2}{4\gamma} \delta^2 + \mathcal{O}^{\text{formal}}(\delta^4).$$

The last term in (39) is actually $\mathcal{O}(\delta^4)/\mathcal{F}(g_\delta)$ so that it is only formally of the fourth order. The rational approximations of $\mathcal{F}(g_\delta)$ and $1/\mathcal{F}(g_\delta)$ are obtained by neglecting all (formal) fourth order terms in (38) and (39). The behavior of $\mathcal{F}(g_\delta)$ for high wave numbers is much better approximated by the rational function than by the Taylor polynomial, see Fig. 3 for a one-dimensional sketch. The approximation of $1/\mathcal{F}(g_\delta)$ is the same as in the polynomial case. The resulting LES model is called the rational LES model.

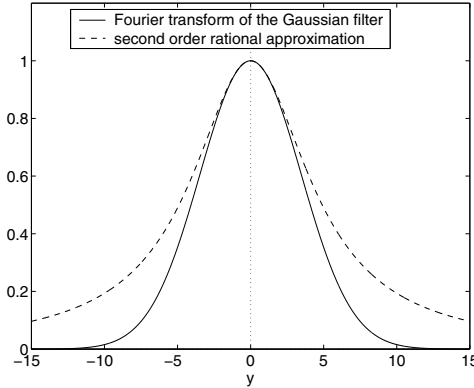


Figure 3. $\mathcal{F}(g_\delta)$ with its second order rational approximation, $\gamma = 6$, $\delta = 1$.

Straightforward calculations with the rational approximation give

$$\begin{aligned} \overline{\mathbf{u} \mathbf{u}^T} &= \left(I - \frac{\delta^2}{4\gamma} \Delta \right)^{-1} (\mathbf{u} \mathbf{u}^T) + \mathcal{O}^{\text{formal}}(\delta^4), \\ \overline{\mathbf{u} \mathbf{u}'^T} &= -\frac{\delta^2}{4\gamma} \left(I - \frac{\delta^2}{4\gamma} \Delta \right)^{-1} (\mathbf{u} \Delta(\mathbf{u})^T) + \mathcal{O}^{\text{formal}}(\delta^4), \\ \overline{\mathbf{u}' \mathbf{u}^T} &= -\frac{\delta^2}{4\gamma} \left(I - \frac{\delta^2}{4\gamma} \Delta \right)^{-1} (\Delta(\mathbf{u}) \mathbf{u}^T) + \mathcal{O}^{\text{formal}}(\delta^4), \\ \overline{\mathbf{u}' \mathbf{u}'^T} &= \mathcal{O}^{\text{formal}}(\delta^4). \end{aligned}$$

Neglecting all $\mathcal{O}^{\text{formal}}(\delta^4)$ terms, applying the inverse Fourier transform and collecting terms leads finally to

$$(40) \quad \mathcal{R}(\mathbf{u}, \mathbf{u}) \approx \frac{\delta^2}{2\gamma} \left(I - \frac{\delta^2}{4\gamma} \Delta \right)^{-1} \nabla \bar{\mathbf{u}} \nabla \bar{\mathbf{u}}^T.$$

In both the Taylor LES model and the rational LES model, the so-called subgrid scale term $\overline{\mathbf{u}'\mathbf{u}'^T}$ is modeled by zero. However, this term is considered to possess great influence on the formation of turbulence. In addition, it turns out in computations that the model zero is insufficient because one obtains in general a blow up of the simulation in finite time, [27], [29]. Proposals for modeling $\overline{\mathbf{u}'\mathbf{u}'^T}$ are of the form $-\nabla \cdot (\nu_T \mathbb{D}(\bar{\mathbf{u}}))$ where ν_T might be the Smagorinsky model (30). Another proposal for ν_T is due to Iliescu and Layton [28]:

$$(41) \quad \nu_T = c_S \delta \left\| \bar{\mathbf{u}} - \left(I - \frac{\delta^2}{4\gamma} \Delta \right)^{-1} \bar{\mathbf{u}} \right\|_2.$$

In the classical LES approach, it is not possible to derive equations for $(\bar{\mathbf{u}}, \bar{p})$ only from the Navier-Stokes equations since a modeling process is also necessary. Thus, the quantities which will be computed using these models will not be $(\bar{\mathbf{u}}, \bar{p})$ but, hopefully good, approximations to $(\bar{\mathbf{u}}, \bar{p})$. To have a clear distinction between the large scale quantities $(\bar{\mathbf{u}}, \bar{p})$ and their approximations, we will denote the solution obtained by the LES models by (\mathbf{w}, r) .

The final LES model based on the approximation of the Fourier transform of the filter function has the form

$$(42) \quad \begin{aligned} \mathbf{w}_t - \nabla \cdot ((2\text{Re}^{-1} + \nu_T) \mathbb{D}(\mathbf{w})) + (\mathbf{w} \cdot \nabla) \mathbf{w} + \nabla r + \nabla \cdot \frac{\delta^2}{2\gamma} (A(\nabla \mathbf{w} \nabla \mathbf{w}^T)) &= \bar{\mathbf{f}} \\ &\text{in } (0, T] \times \Omega, \\ \nabla \cdot \mathbf{w} &= 0 \quad \text{in } [0, T] \times \Omega, \\ \mathbf{w}(0, \cdot) &= \mathbf{w}_0 \quad \text{in } \Omega, \end{aligned}$$

where the operator A depends on the approximation of the Fourier transform of the Gaussian filter:

- $A = I$ for the Taylor LES model (37),
- $A = (I - (\delta^2/(4\gamma))\Delta)^{-1}$ for the rational LES model (40).

For the turbulent viscosity ν_T , the following choices have been presented:

- ν_T is the Smagorinsky model (30),
- ν_T is the Iliescu-Layton model (41).

All derivations so far are performed in \mathbb{R}^d . If the problem is given in a bounded domain, (42) is simply restricted to the domain. However, then the question of

boundary conditions for $(\mathbf{w}, r) \approx (\bar{\mathbf{u}}, \bar{p})$ arises. In the rational LES model (40), one needs also boundary conditions for solving the auxiliary problem

$$-\frac{\delta^2}{4\gamma}\Delta\mathbb{X} + \mathbb{X} = \nabla\mathbf{w}\nabla\mathbf{w}^T.$$

Appropriate boundary conditions for the approximation of the large scales (\mathbf{w}, r) are an open problem. A review of approaches for the treatment of boundaries in LES is given in [47]. There are essentially two approaches:

- impose some form of law-of-the-wall,
- solve numerically a set of simplified equations in the boundary layer region; this is called zonal approach.

The former approach considers the layer on the boundary in a Reynolds averaged sense to impose some wall law. This is justified if the sample of near-wall eddies in a grid cell is sufficiently large. Then, the boundary layer can be assumed to be governed by the RANS equations. For this assumption to hold, the grid size must be very large compared to the Reynolds number. This might be one reason why wall-layer models tend to be more accurate for very high Reynolds numbers.

Zonal approaches are based on the explicit solution of a different set of equations near the boundary. The Two-Layer-Model (TLM) uses two separate grids, a coarse one in the core of the flow and a fine one (refined only in wall-normal direction) on the boundary. On the fine grid, two one-dimensional problems are solved. The so-called Detached Eddy Simulation (DES) uses only one grid. However, RANS equations are solved in the attached boundary layer. The RANS simulations are coupled with LES away from the boundary, see [46] for numerical studies with DES for turbulent channel flows.

The current situation can be summarized as follows:

- Simple models work fairly well on simple problems.
- In more complex configurations, the zonal models give reasonable results. However, there is still much need for improvement.
- No extensive numerical comparisons in complex geometries are available.

For the Smagorinsky model (30) and homogeneous Dirichlet boundary conditions at smooth boundaries, a damping of the constant c_S in a vicinity of the wall is usually applied, the so-called van Driest damping [56], see also [48].

Concerning the auxiliary problem, in [16] it is proposed to use homogeneous Neumann boundary conditions.

3.3.3. Some remarks. There is a huge amount of publications presenting numerical simulations with the Smagorinsky model or the dynamic SGS model, e.g., see [48], [51]. The gradient LES model fails in the form which is presented here. A very fast

blow-up can be observed in simulations, e.g., see [27], [29]. There are modifications of this model which work better. Computations with the rational LES model can be found in [11], [12], [27], [29], [30].

The mathematical analysis of LES models seems to be possible and first results have been already obtained by Guermond et al. [21]. In their paper, two criteria for a rigorous mathematical theory of LES models are proposed: the model should act as a regularization of the Navier-Stokes equations, which leads to a unique weak solution, and it should select a physically relevant solution. It is shown that these criteria are fulfilled by a number of models, e.g., the Navier-Stokes equations with Leray regularization, the Navier-Stokes-alpha model and the Smagorinsky LES model. For models which do not fulfil one of these criteria, e.g., spectral eddy viscosity models, modifications are proposed in [21] such that the new models fulfil both.

In the academic CFD community, LES is considered to be currently among the best performing turbulence models, in particular the dynamic subgrid scale model. However, in industrial applications, LES is often still considered to be too expensive (the computing times are too long) and simpler turbulence models are used.

Advanced LES models have to solve at least two great problems inherited in the classical LES approach:

- modeling of the commutation errors which are committed in the derivation of the space averaged Navier-Stokes equations, in particular if the domain Ω is bounded,
- solving the problem of appropriate boundary conditions for the approximation of the large scales (\mathbf{w}, r) .

4. VARIATIONAL MULTISCALE (VMS) METHODS

Similarly to classical LES methods, VMS methods seek to simulate only large flow structures. Therefore, these methods are also called VMS-LES methods. However, the large scales in a VMS method are defined in a different way than in a classical LES method.

4.1. The basic approach

The difficulties of the classical LES originate in the definition of the large scales by spatial averaging. As an alternative, VMS methods consider large scales which are defined by projection into appropriate spaces. First ideas of projection based methods, also for problems different from the Navier-Stokes equations, can be found in Hughes [24], Guermond [20] and Hughes et al. [23].

Consider the Navier-Stokes equations (1), equipped for simplicity with homogeneous Dirichlet boundary conditions, and a decomposition of the flow into three scales, following [7]:

- the large scales $(\bar{\mathbf{u}}, \bar{p})$,
- the resolved small scales $(\tilde{\mathbf{u}}, \tilde{p})$,
- the unresolved small scales $(\hat{\mathbf{u}}, \hat{p})$,

with $\mathbf{u} = \bar{\mathbf{u}} + \tilde{\mathbf{u}} + \hat{\mathbf{u}}$ and $p = \bar{p} + \tilde{p} + \hat{p}$.

The starting point of a VMS method is the variational formulation of the Navier-Stokes equations. Let $V = (H_0^1(\Omega))^d$ be equipped with the norm $\|\mathbf{v}\|_V = \|\nabla \mathbf{v}\|_{L^2}$ and let $Q = L_0^2(\Omega)$. A variational formulation of (1) reads as follows: Find $\mathbf{u}: [0, T] \rightarrow V$, $p: (0, T] \rightarrow Q$ satisfying for all $(\mathbf{v}, q) \in V \times Q$

$$(43) \quad (\mathbf{u}_t, \mathbf{v}) + (2\text{Re}^{-1} \mathbb{D}(\mathbf{u}), \mathbb{D}(\mathbf{v})) + b(\mathbf{u}, \mathbf{u}, \mathbf{v}) - (p, \nabla \cdot \mathbf{v}) + (q, \nabla \cdot \mathbf{u}) = (\mathbf{f}, \mathbf{v})$$

and $\mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}) \in V$, where $b(\mathbf{u}, \mathbf{v}, \mathbf{w}) = ((\mathbf{u} \cdot \nabla) \mathbf{v}, \mathbf{w})$. Writing (43) in short form

$$A(\mathbf{u}; (\mathbf{u}, p), (\mathbf{v}, q)) = F(\mathbf{v})$$

and decomposing the test functions also into three scales, the variational form of the Navier-Stokes equations can be written as a coupled system: Find $\mathbf{u} = \bar{\mathbf{u}} + \tilde{\mathbf{u}} + \hat{\mathbf{u}}: [0, T] \rightarrow V$, $p = \bar{p} + \tilde{p} + \hat{p}: (0, T] \rightarrow Q$ satisfying for all $(\mathbf{v}, q) \in V \times Q$

$$\begin{aligned} A(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\bar{\mathbf{v}}, \bar{q})) + A(\mathbf{u}; (\tilde{\mathbf{u}}, \tilde{p}), (\bar{\mathbf{v}}, \bar{q})) + A(\mathbf{u}; (\hat{\mathbf{u}}, \hat{p}), (\bar{\mathbf{v}}, \bar{q})) &= F(\bar{\mathbf{v}}), \\ A(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{v}}, \tilde{q})) + A(\mathbf{u}; (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q})) + A(\mathbf{u}; (\hat{\mathbf{u}}, \hat{p}), (\tilde{\mathbf{v}}, \tilde{q})) &= F(\tilde{\mathbf{v}}), \\ A(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\hat{\mathbf{v}}, \hat{q})) + A(\mathbf{u}; (\tilde{\mathbf{u}}, \tilde{p}), (\hat{\mathbf{v}}, \hat{q})) + A(\mathbf{u}; (\hat{\mathbf{u}}, \hat{p}), (\hat{\mathbf{v}}, \hat{q})) &= F(\hat{\mathbf{v}}). \end{aligned}$$

Here, linearity of the variational problem with respect to the test function has been used. Now, the basic ideas and assumptions of a VMS method are as follows:

- the equation with the test function from the unresolved scales is neglected,
- it is assumed that the unresolved scales do not influence the large scales directly, i.e. $A(\mathbf{u}; (\hat{\mathbf{u}}, \hat{p}), (\bar{\mathbf{v}}, \bar{q})) = 0$,
- the influence of the unresolved scales onto the small resolved scales is modeled:

$$A(\mathbf{u}; (\hat{\mathbf{u}}, \hat{p}), (\tilde{\mathbf{v}}, \tilde{q})) \approx B(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q})).$$

The choice of the model $B(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q}))$ has to be guided by physical ideas in turbulence modeling, e.g., eddy viscosity models of Smagorinsky type (30) are often used. From the numerical point of view, the model $B(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q}))$ introduces additional viscosity which acts as stabilization.

Let \bar{V} , \bar{Q} be spaces representing the large scales and \tilde{V} , \tilde{Q} spaces for the resolved small scales. A VMS method reads as a coupled system of the form: Find $(\bar{\mathbf{u}}, \tilde{\mathbf{u}}, \bar{p}, \tilde{p}) \in \bar{V} \times \tilde{V} \times \bar{Q} \times \tilde{Q}$ such that

$$(44) \quad \begin{aligned} A(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\bar{\mathbf{u}}, \bar{p}), (\bar{\mathbf{v}}, \bar{q})) + A(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\tilde{\mathbf{u}}, \tilde{p}), (\bar{\mathbf{v}}, \bar{q})) &= F(\bar{\mathbf{v}}), \\ A(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{v}}, \tilde{q})) + A(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q})) \\ &+ B(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q})) = F(\tilde{\mathbf{v}}) \end{aligned}$$

for or all $(\bar{\mathbf{v}}, \tilde{\mathbf{v}}, \bar{q}, \tilde{q}) \in \bar{V} \times \tilde{V} \times \bar{Q} \times \tilde{Q}$. Note that a characteristic feature of a VMS method is that the model for the influence of the unresolved small scales acts directly only on the resolved small scales. Since the resolved small scales and the large scales are coupled in (44), the model $B(\mathbf{u}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q}))$ influences the large scales indirectly. This is in contrast to classical LES models, where the model acts directly on all resolved scales.

To specify a concrete VMS method, one has to define spaces \bar{V} , \tilde{V} , \bar{Q} , \tilde{Q} and a model $B(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q}))$.

As concerns $B(\bar{\mathbf{u}} + \tilde{\mathbf{u}}; (\bar{\mathbf{u}}, \bar{p}), (\tilde{\mathbf{u}}, \tilde{p}), (\tilde{\mathbf{v}}, \tilde{q}))$, in general the Smagorinsky model (30) or variations of it have been used in literature, see [25], [26], [18], [19], [31].

Concerning finite element methods for discretizing (44), there are at least two principally different approaches. In Gravemeier et al. [18], [19], standard finite element spaces were used for the large scales $\bar{V} \times \bar{Q}$. The finite element spaces $\tilde{V} \times \tilde{Q}$ need to have higher resolution since they should represent small scales. Their approach consists in using mesh cell bubble functions for $\tilde{V} \times \tilde{Q}$, e.g., standard bubbles or residual free bubbles. Therefore, this approach is called the bubble-VMS method. The bubble functions vanish on the faces of the mesh cells, which induces that the resolved small scales cannot cross mesh cell boundaries. This property does not reflect their physical behavior and has given rise to criticism. However, there are no studies available about the impact of this property in numerical simulations. The second way for choosing the spaces consists in using a common standard finite element space for all resolved scales and an additional large scale space. A method of this type was introduced in [31] and will be presented in more detail in Section 4.2.

Numerical studies of VMS methods coupled with spectral methods can be found in [25], [26]. Finite element bubble-VMS methods were used, e.g., in [18], [19] and the coarse space projection-based VMS method in [31].

The principle goal of a VMS method and the dynamic subgrid scale method presented in Section 3.3.1 is similar. Based on the experience that the use of the Smagorinsky model (30) with a fixed constant c_S as turbulence model introduces too much diffusion, one tries to reduce the influence of this model where its application is not necessary. In the dynamic subgrid scale method, this reduction is done

by using a function $c_S(t, \mathbf{x})$ and adjusting this function appropriately. In a VMS method, the reduction is performed by choosing an appropriate small scale space to which the direct influence of the Smagorinsky model is restricted.

4.2. A coarse space projection-based VMS method

Let V^h, Q^h be finite element spaces for the velocity and pressure which fulfil the inf-sup stability condition, i.e., there is a positive constant C independent of the mesh size parameter h such that

$$(45) \quad \inf_{q^h \in Q^h} \sup_{\mathbf{v}^h \in V^h} \frac{(\nabla \cdot \mathbf{v}^h, q^h)}{\|\nabla \mathbf{v}^h\|_{L^2} \|q^h\|_{L^2}} \geq C,$$

let L^H be a finite dimensional space of symmetric $d \times d$ tensor-valued functions defined on Ω and let $\nu_{\text{add}}(V, x)$ be a non-negative function. Then the semi-discrete coarse space projection-based VMS method (continuous in time) is defined as follows: Find $\mathbf{u}^h: [0, T] \rightarrow V^h, p^h: (0, T] \rightarrow Q^h$ and $\mathbb{G}^H: [0, T] \rightarrow L^H$ satisfying

$$(46) \quad A(\mathbf{u}^h; (\mathbf{u}^h, p^h), (\mathbf{v}^h, q^h)) + (\nu_{\text{add}}((\mathbf{u}^h, p^h), h)(\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H), \mathbb{D}(\mathbf{v}^h)) = F(\mathbf{v}^h) \\ \text{for all } (\mathbf{v}^h, q^h) \in V^h \times Q^h, \\ (\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H, \mathbb{L}^H) = 0 \quad \text{for all } \mathbb{L}^H \in L^H.$$

Methods of this kind have been studied in, e.g., [41], [35], [31], [32], [36], [33]. One has to choose two parameters: the additional viscosity $\nu_{\text{add}}((\mathbf{u}^h, p^h), h)$ and the space L^H .

Concerning $\nu_{\text{add}}((\mathbf{u}^h, p^h), h)$, all numerical studies with the method (46) have used the Smagorinsky model (30). A finite element error analysis of (46) for $\nu_{\text{add}}((\mathbf{u}^h, p^h), h) = \nu_{\text{add}}(h)$ can be found in [32].

The other parameter in (46) is the space of symmetric tensors L^H . The second equation in (46) states that the tensor \mathbb{G}^H is just the $L^2(\Omega)$ -projection of $\mathbb{D}(\mathbf{u}^h)$ into L^H : $\mathbb{G}^H = P_{L^H} \mathbb{D}(\mathbf{u}^h)$. With this notation, one can reformulate (46) as follows: Find $\mathbf{u}^h: [0, T] \rightarrow V^h, p^h: (0, T] \rightarrow Q^h$ satisfying

$$(47) \quad A(\mathbf{u}^h; (\mathbf{u}^h, p^h), (\mathbf{v}^h, q^h)) \\ + (\nu_{\text{add}}((\mathbf{u}^h, p^h), h)(I - P_{L^H})\mathbb{D}(\mathbf{u}^h), \mathbb{D}(\mathbf{v}^h)) = F(\mathbf{v}^h)$$

for all $(\mathbf{v}^h, q^h) \in V^h \times Q^h$.

In (46), L^H plays the role of a large scale space such that $(I - P_{L^H})\mathbb{D}(\mathbf{u}^h)$ represents (resolved) small scales of $\mathbb{D}(\mathbf{u}^h)$. To avoid a negative additional viscosity, it is required that $L^H \subset \{\mathbb{D}(\mathbf{v}^h): \mathbf{v}^h \in V^h\}$. In the extreme case when both spaces

coincide, the second term on the left-hand side of (47) vanishes and the Galerkin finite element discretization of the Navier-Stokes equations is recovered. If $L^H = \{\emptyset\}$, one obtains an artificial viscosity stabilization of the Navier-Stokes equations with a possible non-linear artificial viscosity. If $\nu_{\text{add}}((\mathbf{u}^h, p^h), h)$ is the Smagorinsky eddy viscosity model (30), the Smagorinsky LES model is recovered. Since L^H represents large scales, it must be in some sense a coarse finite element space. There are essentially two possibilities. If V^h is a higher order finite element space, L^H can be defined as a low order finite element space on the same grid as V^h . This approach is studied in [31]. The second possibility, in particular if V^h is a low order discretization, consists in defining L^H on a coarser grid, see [33] for a study of this approach in the case of convection-dominated convection-diffusion equations.

Method (46) can be transformed to the standard form (44) of a VMS method, see also [31]. For this purpose, the three-level partitioning given above has to be described by appropriately chosen function spaces. Clearly, the continuous pair of spaces (V, Q) contains all scales. The finite element spaces (V^h, Q^h) contain the large and the resolved small scales. Let $V^H \subset (H^1(\Omega))^d$ be a discrete space such that $L^H = \mathbb{D}(V^H)$. The space V^H should be coarser than V^h . But in the definition of V^H , no boundary conditions, like no-slip conditions, are incorporated. Thus, in general $V^H \not\subset V^h$. The pair of spaces for the large scales is given by (V^H, Q^H) where Q^H is chosen such that an inf-sup condition of type (45) is fulfilled for (V^H, Q^H) . The large scales $P_H \mathbf{u}$ of the velocity are defined by an elliptic projection into V^H and the large scales $P_H p$ of the pressure by the L^2 -projection into Q^H ; $P_H: (V, Q) \rightarrow (V^H, Q^H)$;

$$(48) \quad \begin{aligned} (\mathbb{D}(\mathbf{u} - P_H \mathbf{u}), \mathbb{D}(\bar{\mathbf{v}}^H)) &= 0 \quad \forall \bar{\mathbf{v}}^H \in V^H, \\ (\mathbf{u} - P_H \mathbf{u}, 1) &= 0, \\ (p - P_H p, q^H) &= 0 \quad \forall q^H \in Q^H. \end{aligned}$$

With this definition, a commutation property of the definition of the large scales (by projection) and differentiation can be proved.

Lemma 4.1. *Let $\mathbf{v} \in V$, $L^H = \mathbb{D}(V^H)$ and denote by $P_{L^H} \mathbb{D}(\mathbf{v})$ the L^2 -projection of $\mathbb{D}(\mathbf{v})$ into L^H defined in the second equation of (46). Then*

$$(49) \quad P_{L^H} \mathbb{D}(\mathbf{v}) = \mathbb{D}(P_H \mathbf{v}) \quad \forall \mathbf{v} \in V.$$

Proof. From $L^H = \mathbb{D}(V^H)$ and $P_{L^H} \mathbb{D}(\mathbf{v}) \in L^H$ it follows that there is a $\mathbf{w}^H \in V^H$ such that $P_{L^H} \mathbb{D}(\mathbf{v}) = \mathbb{D}(\mathbf{w}^H)$. Using the second equation of (46) gives

$$(50) \quad (\mathbb{D}(\mathbf{v} - \mathbf{w}^H), \mathbb{L}^H) = 0 \quad \forall \mathbb{L}^H \in L^H.$$

On the other hand, since $L^H = \mathbb{D}(V^H)$, (48) is equivalent to

$$(51) \quad (\mathbb{D}(\mathbf{v} - P_H \mathbf{v}), \mathbb{1}^H) = 0 \quad \forall \mathbb{1}^H \in L^H.$$

The statement of the lemma follows now directly from (50) and (51) since the elliptic projection is unique. \square

Let now ν_{add} be a constant. A straightforward calculation shows that

$$(\nu_{\text{add}}(I - P_{L^H})\mathbb{D}(\mathbf{u}^h), \mathbb{D}(\mathbf{v}^h)) = (\nu_{\text{add}}(I - P_{L^H})\mathbb{D}(\mathbf{u}^h), (I - P_{L^H})\mathbb{D}(\mathbf{v}^h)).$$

Thus, (46) can be reformulated as follows: Find $\mathbf{u}^h: [0, T] \rightarrow V^h$, $p^h: (0, T] \rightarrow Q^h$ satisfying

$$(52) \quad A(\mathbf{u}^h; (\mathbf{u}^h, p^h), (\mathbf{v}^h, q^h)) + (\nu_{\text{add}}(I - P_{L^H})\mathbb{D}(\mathbf{u}^h), (I - P_{L^H})\mathbb{D}(\mathbf{v}^h)) \\ = F(\mathbf{v}^h) \quad \forall (\mathbf{v}^h, q^h) \in V^h \times Q^h.$$

Decompose $V^h = V^H + \tilde{V}^h$, $Q^h = Q^H + \tilde{Q}^h$ with $\tilde{V}^h = (I - P_H)V^h$. It follows from (49) that

$$(I - P_{L^H})\mathbb{D}(\mathbf{v}^h) = \mathbb{D}(\mathbf{v}^h - P_H \mathbf{v}^h) = \mathbb{D}((I - P_H)\mathbf{v}^h) = \mathbb{D}(\tilde{\mathbf{v}}^h).$$

The decompositions $\mathbf{u}^h = \bar{\mathbf{u}}^H + \tilde{\mathbf{u}}^h$, $p^h = \bar{p}^H + \tilde{p}^h$, $\mathbf{v}^h = \bar{\mathbf{v}}^H + \tilde{\mathbf{v}}^h$ and $q^h = \bar{q}^H + \tilde{q}^h$ are inserted into (52) together with using the linearity of $A(\cdot; \cdot, \cdot)$ with respect to the second and third component. Writing the arising equation formally as a coupled system gives

$$(53) \quad A(\bar{\mathbf{u}}^H + \tilde{\mathbf{u}}^h; (\bar{\mathbf{u}}^H, \bar{p}^H), (\bar{\mathbf{v}}^H, \bar{q}^H)) \\ + A(\bar{\mathbf{u}}^H + \tilde{\mathbf{u}}^h; (\tilde{\mathbf{u}}^h, \tilde{p}^h), (\bar{\mathbf{v}}^H, \bar{q}^H)) = F(\bar{\mathbf{v}}^H)$$

for all test functions $(\bar{\mathbf{v}}^H, \bar{q}^H) \in V^H \times Q^H$ and

$$(54) \quad A(\bar{\mathbf{u}}^H + \tilde{\mathbf{u}}^h; (\bar{\mathbf{u}}^H, \bar{p}^H), (\tilde{\mathbf{v}}^h, \tilde{q}^h)) + A(\bar{\mathbf{u}}^H + \tilde{\mathbf{u}}^h; (\tilde{\mathbf{u}}^h, \tilde{p}^h), (\tilde{\mathbf{v}}^h, \tilde{q}^h)) \\ + (\nu_{\text{add}}\mathbb{D}(\tilde{\mathbf{u}}^h), \mathbb{D}(\tilde{\mathbf{v}}^h)) = F(\tilde{\mathbf{v}}^h)$$

for all test functions from $\tilde{V}^h \times \tilde{Q}^h$. The coupled system (53), (54) possesses exactly the form (44). The unresolved scales are modeled only in the small scale equation (54) with the model

$$B(\mathbf{u}^h; (\bar{\mathbf{u}}^H, \bar{p}^H), (\tilde{\mathbf{u}}^h, \tilde{p}^h), (\tilde{\mathbf{v}}^h, \tilde{q}^h)) = (\nu_{\text{add}}\mathbb{D}(\tilde{\mathbf{u}}^h), \mathbb{D}(\tilde{\mathbf{v}}^h))$$

and this model influences the large scales solely indirectly by the coupling of (53) and (54).

5. CONCLUDING REMARKS

The reliable and fast numerical simulation of turbulent flows is still a big challenge in applications. Simulations in industrial applications use in general traditional approaches like Reynolds averaged Navier-Stokes equations (RANS) or k - ε -type models.

LES, which is currently the most popular way of turbulence modeling in the scientific CFD community, is still considered to be too expensive. This situation can be changed only if more efficient algorithms for LES simulations are developed. This includes, in particular, adaptive discretizations (in time and space) and fast solvers (multigrid-based). Also, the use of parallel computers, which are easily available nowadays, offers an opportunity to increase the efficiency of LES simulations considerably.

The development of VMS methods is yet at the beginning. This approach still has to be studied for benchmark problems available and to be compared to other turbulence modeling approaches. There is a large potential of improvement in the nowadays used VMS methods if it becomes possible to define the additional space (coarse or fine, depending on the realization) and the additional viscosity adaptively using a posteriori information.

There are many open mathematical problems concerning turbulence models. Some of them are the existence and uniqueness of solutions, e.g., for the rational LES model, and the error analysis for fully (in time and space) discretized models.

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Author's address: V. John, FR 6.1–Mathematik, Universität des Saarlandes, Postfach 15 11 20, 66041 Saarbrücken, Germany, e-mail: john@math.uni-sb.de.