ON DUALITY BASED A POSTERIORI ERROR ESTIMATION IN VARIOUS NORMS AND LINEAR FUNCTIONALS FOR LES

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Abstract. We derive a posteriori error estimates for the filtered velocity field in a LES, in various norms and linear functionals. The a posteriori error estimates take the form of an integral in space-time of a discretization residual and a modeling residual times a dual weight. The discretization residual is directly computable, and the modeling residual is estimated by a scale similarity model. We approximate the dual weight by solving an associated linearized dual problem numerically. Computational examples from transition to turbulence in Couette flow are presented.

Key words. adaptive finite element methods, duality, a posteriori error estimates, turbulent viscous incompressible flow, large eddy simulation

AMS subject classifications. 65M60, 76F65

1. Introduction. In this paper we investigate a posteriori error estimation for adaptive finite element methods, using duality techniques, for turbulent viscous incompressible flow, in the case we are not able to resolve all scales of motion in a Direct Numerical Simulation DNS.

A posteriori error estimation is traditionally done with respect to an energy-norm, naturally induced by the underlying differential operator, resulting in estimates in terms of computable residuals. For surveys and references on this approach we refer to [38, 1]. Unfortunately, in most applications the energy-norm does not provide useful bounds on the error in quantities of real physical interest. Another approach is to use duality arguments to obtain bounds on the error in other norms, such as the $L_2$-norm, or the error in various functionals of the solution, such as drag or lift forces for example. The idea of using duality arguments in a posteriori error estimation goes back to Babuška and Miller [2, 3, 4] in the context of postprocessing ‘quantities of physical interest’ in elliptic model problems. A framework for more general situations has since then been systematically developed by Eriksson & Johnson and Becker & Rannacher, with coworkers, see e.g. [13, 11, 5, 6, 31, 32]. For a detailed account of the development and application of this framework we refer in particular to the review papers [11, 6] and the references therein.

In fluid mechanics, applications of adaptive finite element methods based on this framework have been increasingly advanced, with computations of functionals such as drag and lift forces and pressure differences, for 2d laminar benchmark problems in [5, 17], and for 3d laminar benchmark problems in [22]. The next natural step is to extend these methods to turbulent flows, where we are not able to resolve all scales of motion in a computation. In particular, we want to extend to Large Eddy Simulation LES, where we apply a spatial averaging operator, or filter, to the Navier-Stokes equations to obtain a new set of equations for the averaged (or filtered) variables.

Such an averaging process involves several mathematical issues that has to be addressed; such as a possible commutation error if the filter does not commute with differentiation, finding the correct boundary conditions for the filtered variables, and the problem of closure due to filtering of the non linear term in the Navier-Stokes equations. There is an extensive amount of work on LES, in particular regarding the
closure problem and the choice of subgrid models, and we refer to [16, 36] and the references therein for details. The commutation error is investigated in [10, 37], for example, and for work on boundary conditions (or near wall models) for LES we refer to [30, 34] and the references therein.

In this paper we focus on a posteriori error estimation for LES, where we use stabilized finite element methods to discretize the filtered equations. The a posteriori error estimates take into consideration both the numerical error from discretization of the filtered Navier-Stokes equations, and the modeling error from unresolved subgrid scales. We bound the error in various norms and linear functionals of the computed finite element solution, with respect to the filtered velocity, in terms of an integral in space-time of a discretization residual and a modeling residual times a dual weight. The dual weight is obtained by solving an associated linearized dual problem, and contains information about error propagation in space-time. If we use a subgrid model in the computation, the subgrid modeling error is included in the a posteriori error estimates, which opens the possibility of comparing the error using different subgrid models. Altogether, the a posteriori error estimates open the possibility of adaptively choosing both an optimal mesh and an optimal subgrid model.

This approach to a posteriori error estimation with respect to the averaged solution, using duality techniques, in terms of a modeling error and a discretization error was developed for convection-diffusion-reaction equations in [18, 27, 23, 19, 20].

Related approaches with a posteriori error estimates in terms of a modeling and a discretization contribution to the total error have been suggested. For example, more recently in [7] similar ideas are presented with applications to 2d convection-diffusion-reaction problems, and in [14] the notion of a modeling error is present in a framework for defect-correction with application to the stationary Navier-Stokes equations in 2d, although the estimates bound the error with respect to the unfiltered solution as opposed to the approach in this paper where we aim for error control with respect to the filtered solution. A posteriori error estimation with respect to spatial averages in the Navier-Stokes equations is considered in [9, 8], where it is shown that for the stationary Navier-Stokes equations, under the restrictive assumption of strong stability for the corresponding dual problem, the filtered error converges of higher order than the unfiltered error in $L_2$-norm.

To the best knowledge of the author, this paper represents the first presentation of a posteriori error estimates with respect to a filtered solution of the turbulent Navier-Stokes equations in 3d, of the form discretization and modeling residuals times dual weights, with numerical approximation of the dual weights through computation of time dependent linearized dual Navier-Stokes equations in 3d.

The discretization residual is directly computable from the approximate solution, whereas the modeling residual needs to be estimated. In this paper we use a scale similarity subgrid model to estimate the modeling residual. A key issue for the a posteriori error estimates to be useful is then the size of the dual weights.

The linearized dual Navier-Stokes equations is a system of linear convection-diffusion-reaction equations with the components of the gradient of the computed solution acting as reaction coefficients. Thus the dual problem seems potentially very dangerous. In particular, standard analytical estimates based on Grönwall’s inequality suggest that perturbations grow exponentially. The key result of this paper is that the computational solutions of these dual problems indicate that in the turbulent flow considered in this paper certain mean value output quantities, corresponding to regular data in the dual problem, are computable to a reasonable computational cost.
In continuations of this paper we use the a posteriori error estimates in this paper for adaptive finite element methods for LES [21], which is then extended to Adaptive DNS/LES in [26].

In Section 2 we present the Navier-Stokes equations as a model for viscous incompressible flow, and we state the discretization of the LES equations using the $G^2$-method, and in particular the $cG(1)cG(1)$-method. In Section 3 we present a posteriori error estimates for the $cG(1)cG(1)$-method, and in Section 4 we compute the a posteriori error bounds for a turbulent test problem, solving the 3d time dependent linearized dual Navier-Stokes equations with various data. From the numerical tests we make some observations, and we conclude with a summary and some remarks on future directions.

2. Discretization of the averaged Navier-Stokes equations. The incompressible Navier-Stokes equations expressing conservation of momentum and incompressibility of a unit density constant temperature Newtonian fluid with constant kinematic viscosity $\nu > 0$ enclosed in a volume $\Omega$ in $\mathbb{R}^3$ (where we assume that $\Omega$ is a polygonal domain) with homogeneous Dirichlet boundary conditions, take the form: Find $(u,p)$ such that

$$\begin{align*}
\dot{u} + (u \cdot \nabla)u - \nu \Delta u + \nabla p &= f & \text{in } \Omega \times I, \\
\nabla \cdot u &= 0 & \text{in } \Omega \times I, \\
\nabla \cdot u &= 0 & \text{on } \partial \Omega \times I, \\
u \Delta u &= u(\cdot,0) = u_0 & \text{in } \Omega,
\end{align*}$$

(2.1)

where $u(x,t) = (u_i(x,t))$ is the velocity vector and $p(x,t)$ the pressure of the fluid at $(x,t)$, and $f$, $u_0$, $I = (0,T)$ is a given driving force, initial data and time interval, respectively. The quantity $\nu \Delta u - \nabla p$ represents the total fluid force, and may alternatively be expressed as

$$\nu \Delta u - \nabla p = \text{div } \sigma(u,p),$$

where $\sigma(u,p) = (\sigma_{ij}(u,p))$ is the stress tensor, with components $\sigma_{ij}(u,p) = 2\nu \epsilon_{ij}(u) - p \delta_{ij}$, composed of the stress deviatoric $2\nu \epsilon_{ij}(u)$ with zero trace and an isotropic pressure: here $\epsilon_{ij}(u) = (u_{i,j} + u_{j,i})/2$ is the strain tensor, with $u_{i,j} = \partial u_i/\partial x_j$, and $\delta_{ij}$ is the usual Kronecker delta, the indices $i$ and $j$ ranging from 1 to 3. We assume that (2.1) is normalized so that the reference velocity and typical length scale are both equal to one. The Reynolds number $Re$ is then equal to $\nu^{-1}$.

2.1. The averaged Navier-Stokes equations. In a turbulent flow we may not be able to resolve all scales computationally. We may instead aim at computing a running average $u^h$ of $u$ on a scale $h$, defined by

$$u^h(x,t) = \frac{1}{h^3} \int_{Q_h} u(x+y,t) \, dy,$$

(2.2)

where $h = h(x)$ and $Q_h = \{ y \in \mathbb{R}^3 : |y_i| \leq h/2 \}$. In the LES literature it is common to define the averaging operator through convolution by a certain filter function, and there is a multitude of filter functions being used. Filtering on bounded domains may introduce commutation errors, which is investigated for example in [10, 37]. In this paper we focus on a posteriori error estimation, and ignore possible commutation errors. Though we only consider the case of the so called box filter corresponding to (2.2) in this paper, the techniques for a posteriori error estimation are general and
apply to other filters, possibly with modifications for commutation errors associated with such filters.

If we take the running average of the equations (2.1), corresponding to LES, we obtain the following equations for $u^h$:

\[\begin{align*}
\dot{u}^h + (u^h \cdot \nabla)u^h - \nu \Delta u^h + \nabla p^h + F_h(u) &= f^h \quad \text{in } \Omega \times I, \\
\nabla \cdot u^h &= 0 \quad \text{in } \Omega \times I, \\
u \frac{\partial u^h}{\partial t} &= 0 \quad \text{on } \partial \Omega \times I, \\
u \frac{\partial u^h}{\partial t}(\cdot, 0) &= u_0^h \quad \text{in } \Omega,
\end{align*}\]

(2.3)

where we choose homogeneous Dirichlet boundary conditions for $u^h$. $F_h(u) = \nabla \cdot \tau^h(u)$, and $\tau^h_{ij}(u) = (u_i u_j)^h - u_i^h u_j^h$ is the Reynolds stress tensor. The closure problem of LES is how to model $F_h(u)$ in terms of $u^h$ in a subgrid model $\hat{F}_h(u^h)$, or $\tau^h(u)$ in a model $\hat{\tau}_h(u^h)$. In this paper we focus on a posteriori error estimation, and we refer to [16, 36] and the references therein for work on subgrid modeling for LES, and [30, 34] for work on boundary conditions for LES.

A weak formulation of (2.3) reads: find $(u^h, p^h) \in L_2(I; [H^1_0(\Omega)]^3 \times L_2(\Omega))$, with $\dot{u}^h \in L_2(I; [L_2(\Omega)]^3)$, such that

\[\begin{align*}
(\dot{u}^h + u^h \cdot \nabla u^h, v) + (\nu \nabla u^h, \nabla v) - (p^h, \nabla \cdot v) \\
- (\tau^h(u), \nabla v) + (\nabla \cdot u^h, q) &= (f^h, v),
\end{align*}\]

(2.4)

for all $(v, q) \in L_2(I; [H^1_0(\Omega)]^3 \times L_2(\Omega))$, where we assume that $f^h \in L_2(I; [L_2(\Omega)]^3)$.

$L_2(\Omega)$ is the Hilbert space of Lebesgue square integrable functions on $\Omega$, with scalar product $(\cdot, \cdot)$ and norm $\|\cdot\|$, and $H^s(\Omega)$ is the standard Hilbert space of functions in $L_2(\Omega)$ with also partial derivatives of order $\leq s$ in $L_2(\Omega)$. $H^s_0(\Omega)$ denotes the functions $v \in H^s(\Omega)$ that satisfies the Dirichlet boundary condition $v|_{\partial \Omega} = 0$ (in the sense of traces), and in particular $H^1_0(\Omega)$ denotes the functions in $H^1(\Omega)$ that vanish on $\partial \Omega$. We further let $C(I; X)$ denote the space of all continuous functions $v : I \to X$, with $\sup_{t \in I} \|v(t)\|_X < \infty$, where $X$ denotes a Banach space with norm $\|\cdot\|_X$.

2.2. The G\(^2\)-method for turbulent flow. For a survey and references for finite element methods for the incompressible Navier-Stokes equations, see [35]. Here we state the G\(^2\)-method for homogeneous Dirichlet boundary conditions, for details see e.g. [24].

Let $0 = t_0 < t_1 < ... < t_N = T$ be a sequence of discrete time steps with associated time intervals $I_n = (t_{n-1}, t_n]$ of length $k_n = t_n - t_{n-1}$ and space-time slabs $S_n = \Omega \times I_n$, and let $W_n \subset H^1(\Omega)$ be a finite element space consisting of continuous piecewise polynomials of degree $p$ on a mesh $T_n = \{K\}$ of mesh size $h_n(x)$ with $W_0$ the functions in $W_n$ vanishing on $\partial \Omega$. To define the G\(^2\)-method for homogeneous Dirichlet boundary conditions for the velocity, let for a given velocity field $\beta$ on $S_n = \Omega \times I_n$ vanishing on $\partial \Omega \times I_n$, the particle paths $x(\bar{x}, \bar{t})$ be defined by

\[\frac{dx}{dt} = \beta(x, t) \quad \bar{t} \in I_n, \quad \text{and} \quad x(\bar{x}, t_n) = \bar{x}, \quad \bar{x} \in \Omega,
\]

(2.5)

and introduce the corresponding mapping $F^\beta_n : S_n \to S_n$ defined by $(x, t) = F^\beta_n(\bar{x}, \bar{t}) = \beta(x, t)$.
where \( x(x, \tilde{t}, \tilde{\ell}) \) satisfies (2.5). Define for a given \( q \geq 0 \) the spaces

\[
\bar{V}_n^\beta = \{ \bar{v} \in H^1(S_n)^3 : \bar{v}(\bar{x}, \bar{\ell}) = \sum_{j=0}^q (\ell - t_n)U_j(\bar{x}), U_j \in [W_{0n}]^3 \},
\]

\[
\bar{Q}_n^\beta = \{ \bar{q} \in H^1(S_n) : \bar{q}(\bar{x}, \bar{\ell}) = \sum_{j=0}^q (\ell - t_n)q_j(\bar{x}), q_j \in W_n \},
\]

together with their analogs in \((x, t)\)-coordinates: \( V_n^\beta = \{ v : \bar{v} \in \bar{V}_n^\beta \}, Q_n^\beta = \{ q : \bar{q} \in \bar{Q}_n^\beta \}, \) where \( v(x, t) = \bar{v}(\bar{x}, \bar{\ell}) \) and \( q(x, t) = \bar{q}(\bar{x}, \bar{\ell}) \). Defining finally \( V^\beta \times Q^\beta = \prod_{n=1}^N V_n^\beta \times Q_n^\beta \), we can now formulate the \( G^2 \)-method for (2.3) as follows: Find \((U_h, P_h) \in V^\beta \times Q^\beta \), such that for \( n = 1, 2, \ldots, N \),

\[
\begin{aligned}
(\bar{U}_n + (U_h \cdot \nabla)U_h, v)_n - (P_h, \nabla \cdot v)_n + (q, \nabla \cdot U_h)_n + (2\nu c(U_h), \epsilon(v))_n \\
- (\hat{\tau}^h(U_h), \nabla v)_n + (\delta_1 a(U_h; H_h, P_h), a(U_h; v, q))_n + (\delta_2 \nabla \cdot U_h, \nabla \cdot v)_n \\
+ ([U_h^{n-1}], v_n^{n-1} - \bar{v}^t) \quad \forall v, q \in V_n^\beta \times Q_n^\beta,
\end{aligned}
\]

where \( a(w; v, q) = D_{w,v}v + \nabla q - \nu \Delta v \) with the Laplacian defined elementwise, \( \delta_1 = \frac{1}{2}(k-1 + [U]^2h^{-2}n^{-2})^{-1/2} \) in the convection-dominated case \( \nu < U_h^n \) and \( \delta_1 = \kappa_1 h^2 \) otherwise, \( \delta_2 = \kappa_2 h \) if \( \nu < U_h^n \) and \( \delta_2 = \kappa_2 h^2 \) otherwise, with \( \kappa_1 \) and \( \kappa_2 \) positive constants of unit size, and

\[
(\nu, w)_n = \int_{t_n} \int_{t_n} (v, w) dt, \quad (v, w) = \sum_{k \in T_n} \int_K v \cdot w dx,
\]

\[
(\epsilon(v), \epsilon(w)) = \sum_{i,j=1}^3 \left( e_{ij}^+(v), e_{ij}^-(w) \right), \quad (\hat{\tau}^h(v), \nabla w) = \sum_{i,j=1}^3 \left( \hat{\tau}_{ij}^h(v), \partial w_i / \partial x_j \right).
\]

Further, \([v^n] = v_n^t - v_n^s\) is the jump across the time level \( t_n \) with \( v_n^t \) the limit from \( t > t_n \) and \( v_n^s \) the limit from \( t < t_n \). In the Eulerian streamline diffusion method we choose \( \beta = 0 \), which means that the mesh does not move in time. The characteristic Galerkin method is obtained by choosing \( \beta = U \) (and then \( \delta_1 = \kappa_1 h^2 \)), which means that the mesh moves with the fluid particles. We may also choose \( \beta \) differently which gives various versions of ALE-methods, with the mesh and particle velocity being (partly) different; for example we may move the mesh with the particle velocity at a free boundary, while allowing the mesh to move differently inside the domain.

Note that the viscous term \((2\nu c(U), \epsilon(v))_n\) may alternatively occur in the form \((\nu \nabla U, \nabla v)_n = \sum_{i=1}^3 (\nu \nabla U_i, \nabla v_i)_n\). In the case of Dirichlet boundary conditions the corresponding variational formulations are equivalent, but not so in the case of Neumann boundary conditions.

2.3. The cG(1)cG(1)-method for turbulent flow. The cG(1)cG(1)-method is a variant of the above \( G^2 \)-method using the continuous Galerkin method cG(1) in time instead of a discontinuous Galerkin method. With cG(1) in time the trial functions are continuous piecewise linear and the test functions piecewise constant. cG(1) in space corresponds to both test functions and trial functions being continuous piecewise linear. The cG(1)cG(1)-method for the averaged Navier-Stokes equations (2.3), with homogeneous Dirichlet boundary conditions, reads: For \( n = 1, \ldots, N \), find
\((U_h^n, P^n_h) \in W_{\text{on}}^3 \times W_n\), such that

\[
\begin{align*}
&((U_h^n - U_h^{n-1})k_n^{-1}, v) + (\hat{U}_h^n \cdot \nabla \hat{U}_h^n + \nabla P^n_h, v + \delta_1 (\hat{U}_h^n \cdot \nabla v + \nabla q)) \\
&+ (\delta_2 \nabla \cdot \hat{U}_h^n, \nabla v) + (\nabla \cdot \hat{U}_h^n, q) + (v \nabla \hat{U}_h^n, \nabla v) - (\hat{\tau}_h^n(\hat{U}_h^n), \nabla v) \\
&= (f^n, v + \delta_1 (\hat{U}_h^n \cdot \nabla v + \nabla q)) \quad \forall (v, q) \in W_{\text{on}}^3 \times W_n,
\end{align*}
\]

where \(\hat{U}_h^n = \frac{1}{2} (U_h^n + U_h^{n-1})\). The modification for using non homogeneous Dirichlet boundary conditions is straightforward, with the non homogeneous Dirichlet boundary conditions incorporated in the trial space.

This method corresponds to a second order accurate Crank-Nicolson time-stepping, but the stabilization suffers from an inconsistency up to the term \(\delta_1 \hat{u}\) resulting from using piecewise constant test functions. The inconsistency seems to be acceptable unless \(\hat{u}\) is large, and we use \(cG(1)cG(1)\) in the computations presented below.

3. A posteriori error estimation for LES. Aiming at error control of the quantity \(g(u_h - U_h)\), defined by

\[
\begin{align*}
g(w) &= \int_Q w \cdot \psi \, dx \, dt, \\
\end{align*}
\]

for \(w \in L^2(I; [L^2(\Omega)]^3)\) in \(Q = \Omega \times I\), with \(\psi \in L^2(I; [L^2(\Omega)]^3)\) given, we introduce the following linearized dual problem: Find \((\varphi, \theta) \in L^2(I; [H^1_0(\Omega)]^3 \times H^2(\Omega))\), with \((\hat{\varphi}, \hat{\theta}) \in C(I; [H^1(\Omega)]^3 \times L^2(\Omega))\), such that

\[
\begin{align*}
-\hat{\varphi} - (u_h \cdot \nabla)\varphi + \nabla U_h \cdot \varphi + \nabla \theta - \nu \Delta \varphi &= \psi \quad \text{in } Q, \\
\nabla \cdot \varphi &= 0 \quad \text{in } Q, \\
\varphi &= 0 \quad \text{on } \Gamma \times I, \\
\varphi(\cdot, T) &= 0 \quad \text{in } \Omega,
\end{align*}
\]

where \((\nabla U_h \cdot \varphi)_j = (U_h)_j \cdot \varphi\). We assume that there exist a unique solution to (3.2), and we note that for the corresponding weak formulation of (3.2) to make sense, we would only need that \((\varphi, \theta) \in L^2(I; [H^1_0(\Omega)]^3 \times L^2(\Omega))\) and \(\varphi \in L^2(I; [L^2(\Omega)]^3)\). The extra regularity is needed for the interpolation error estimates in the proof of the a posteriori error estimate in Theorem 3.4.

Depending of the choice of \(\psi\), the quantity \(g(u_h - U_h)\) may represent various norms of the error \(u_h - U_h\) or, by Riesz representation theorem, the error in any linear functional \(g(u_h)\), such as point values or mean values of \(u_h\), for example.

Other possibilities of target functionals are possible. For example, if we are interested in norms or functionals of the error in the pressure we choose a non zero source term in the second equation in (3.2) instead, and for functionals involving surface integrals, such as drag and lift forces, we have a non zero boundary condition in (3.2). A non zero final condition in (3.2) corresponds to an error estimate involving the error at time \(T\). For a posteriori error estimates corresponding to various data in the dual problem, see [22].

3.1. Discretization errors and modeling errors. To derive a posteriori error estimates for the averaged Navier-Stokes equations, we have to take into account both the numerical error from the discretization of (2.3) and the modeling error from the approximation of \(F_h(u)\) in (2.3).

Lemma 3.1 (Error representation for the \(G^2\)-method). With \(u^h\) the solution to (2.3), and \(\psi \in L^2(I; [L^2(\Omega)]^3)\) given, we have the following error representation
formula for all \((U_h, P_h) \in V^\beta \times Q^\beta:\)

\[
\int_Q (u^h - U_h) \cdot \psi \, dx \, dt = \sum_{n=1}^{N} \left\{ (\hat{\tau}^h(U_h) - \nu \nabla U_h, \nabla \varphi)_n + (f^h - \hat{U}_h - (U_h \cdot \nabla)U_h, \varphi)_n \right. \\
+ (\nabla \cdot U_h, \theta)_n + (P_h, \nabla \cdot \varphi)_n + (\tau^h(u) - \hat{\tau}^h(U_h), \nabla \varphi)_n - \sum_{n=1}^{N-1} ([U^n_h], \varphi(t_n)),
\]

where \((\varphi, \theta)\) is the solution to the dual problem (3.2).

Proof. We multiply the first equation of (3.2) by \(e = u^h - U_h\), then integrate over \(Q\) together with integration by parts, using that \((u^h \cdot \nabla)u^h - (U_h \cdot \nabla)U_h = (u^h \cdot \nabla)e + (e \cdot \nabla)U_h\) with \(e\) vanishing on \(\partial \Omega\), to get

\[
\int_Q e \cdot \psi \, dx \, dt = \sum_{n=1}^{N} \left\{ (\hat{e} + (u^h \cdot \nabla)e + (e \cdot \nabla)U_h, \varphi)_n - (\nabla \cdot e, \theta)_n \right.
\]

\[
+ (\nu \nabla e, \nabla \varphi)_n - (p^h - P_h, \nabla \cdot \varphi)_n \right. \\
- \sum_{n=1}^{N-1} ([U^n_h], \varphi(t_n))
\]

\[
= \sum_{n=1}^{N} \left\{ (\hat{u}^h + (u^h \cdot \nabla)u^h, \varphi) + (\nu \nabla u^h, \nabla \varphi)_n - (p^h, \nabla \cdot \varphi)_n - (\nabla \cdot u^h, \theta) + (\nabla \cdot U_h, \theta)_n \\
- (\hat{U}_h + (U_h \cdot \nabla)U_h, \varphi) - (\nu \nabla U_h, \nabla \varphi)_n + (P_h, \nabla \cdot \varphi)_n \right. \right. \\
- \sum_{n=1}^{N-1} ([U^n_h], \varphi(t_n)).
\]

We add and subtract the subgrid model term \((\hat{\tau}^h(U_h), \nabla \varphi)_n\), and then we use the weak formulation (2.4).

\[
\square
\]

In the rest of this paper we will refer to the part of the error in Lemma 3.1 that corresponds to the \(G^2\)-method (2.6), with \(\delta_1 = \delta_2 = 0\), as the discretization error. The other part of the error in Lemma 3.1, that corresponds to the difference in the true Reynolds stresses and the subgrid model evaluated at the finite element solution \(U_h\), we refer to as the modeling error.

The above definitions are non standard in the LES literature, where the modeling error refers to the difference between averages of solutions to the Navier-Stokes equations and the exact solution to the LES equations, and the discretization error refers to the difference between the exact solution to the LES equations and the numerical approximation to the LES equations.

### 3.2. A posteriori error estimation for the \(cG(1)cG(1)\)-method.

We note that Lemma 3.1 is valid for any \((U_h, P_h) \in V^\beta \times Q^\beta\). If \((U_h, P_h)\) is the solution to a Galerkin method, for example the \(cG(1)cG(1)\)-method (2.7) with \(\delta_1 = \delta_2 = 0\), then we may use the Galerkin orthogonality property of (2.7) to subtract interpolants \((\hat{\Phi}, \hat{\Theta}) \in W^3_0 \times W^n\) (piecewise constant in time) of the dual solution \((\varphi, \theta)\), to estimate the interpolation errors in terms of derivatives of \((\varphi, \theta)\) and powers of the space and time discretization parameters.

For simplicity, we present the corresponding a posteriori error estimate for the \(cG(1)cG(1)\)-method with \(\delta_1 = \delta_2 = 0\). For the case \(\delta_1, \delta_2 \neq 0\), we would adjust the
dual problem (3.2) to be the transposition of the linearized variational form corresponding to the stabilized method, which is beyond the scope of this paper. In [28], the choice of different dual problems for stabilized finite element methods is investigated, in the case of linear problems.

To estimate the interpolation error \( \varphi - \Phi \) over the space-time domain \( \Omega \times I_n \), we introduce \( \bar{\varphi} \), a temporal average of \( \varphi \) over \( I_n \), defined by

\[
\bar{\varphi}(x) = \frac{1}{k_n} \int_{I_n} \varphi(x, s) \, ds,
\]

and we also introduce the following definitions:

\[
(v, w)_K = \int_K v \cdot w \, dx, \quad (v, w)_{\partial K} = \int_{\partial K} v \cdot w \, ds,
\]

\[
\|v\|_K = (v, v)_K^{1/2}, \quad \|v\|_{\partial K} = (v, v)_{\partial K}^{1/2},
\]

\[
|v|_K = (|v_1|_K, |v_2|_K, |v_3|_K), \quad |v|_{\partial K} = (|v_1|_{\partial K}, |v_2|_{\partial K}, |v_3|_{\partial K}),
\]

\[
|v|_K,\infty = (\sup_{\eta \in \mathcal{I}_n} |v_1(\eta)|_K, \sup_{\eta \in \mathcal{I}_n} |v_2(\eta)|_K, \sup_{\eta \in \mathcal{I}_n} |v_3(\eta)|_K),
\]

\[
|v|_{\partial K,\infty} = (\sup_{\eta \in \mathcal{I}_n} |v_1(\eta)|_{\partial K}, \sup_{\eta \in \mathcal{I}_n} |v_2(\eta)|_{\partial K}, \sup_{\eta \in \mathcal{I}_n} |v_3(\eta)|_{\partial K}),
\]

with the obvious simplifications for scalar functions \( v \) and \( w \). To prove Theorem 3.4, we use Lemma 3.1 together with the following two lemmas:

**Lemma 3.2.** For \( (v, w) \in L^2(I_n; [L_2(\Omega)]^2 \times L_2(\Omega)) \), \( (\varphi, \theta) \in L^2(I_n; [H^2_0(\Omega)]^2 \times H^2(\Omega)) \), with \( (\bar{\varphi}, \bar{\theta}) \in C(I_n; [L_2(\Omega)]^2 \times L_2(\Omega)) \), and \( (\Phi, \Theta) \in W^3_n \times W^3_n \) constant in time, we have

\[
|(v, \varphi - \Phi)_n| \leq \int_{I_n} \sum_{K \in \mathcal{T}_n} \|v\|_K \cdot (C_{n,K} k_n |\bar{\varphi}|_K,\infty + C_{n,K} h_n^2 |\bar{\varphi}|_K) \, dt,
\]

\[
|(w, \theta - \Theta)_n| \leq \int_{I_n} \sum_{K \in \mathcal{T}_n} \|w\|_K (C_{n,K} k_n |\bar{\theta}|_K,\infty + C_{n,K} h_n^2 |\bar{\theta}|_K) \, dt,
\]

where \( h_{n,K} \) is the diameter of element \( K \in \mathcal{T}_n \), and \( D^2 \) measures second order derivatives with respect to \( x \).

**Proof.** We prove the first inequality:

\[
|(v, \varphi - \Phi)_n| \leq |(v, \varphi - \bar{\varphi})_n| + |(v, \bar{\varphi} - \Phi)_n| = I_1 + I_2.
\]

Using the mean value theorem, with \( \eta, \zeta \in I_n \), we get for \( (x, t) \in \Omega \times I_n \) that

\[
\varphi(x, t) - \bar{\varphi}(x) = \varphi(x, t) - \varphi(x, \zeta) = \dot{\varphi}(x, \eta)(t - \eta) \leq C k_n \sup_{\eta \in I_n} |\dot{\varphi}(x, \eta)|. \tag{3.5}
\]

Cauchy-Schwarz inequality on each element gives

\[
I_1 \leq \int_{I_n} \sum_{K \in \mathcal{T}_n} \|v\|_K \cdot (C_{n,K} k_n \sup_{\eta \in I_n} |\dot{\varphi}(\eta)|_K) \, dt.
\]

For \( I_2 \), both \( \bar{\varphi} \) and \( \Phi \) are constant in time. We first use Cauchy-Schwarz inequality on each element, and then a standard interpolation estimate in \( x \) of the form \( \|h_{n,K}(\bar{\varphi} - \Phi_t)\|_K \leq C \|D^2 \bar{\varphi}\|_K \), for each \( t \in I_n \), to get

\[
I_2 \leq \int_{I_n} \sum_{K \in \mathcal{T}_n} |v|_K \cdot (C_{n,K} h_{n,K}^2 |D^2 \bar{\varphi}|_K) \, dt.
\]
The proof of the second inequality in the lemma is similar to the proof of the first inequality.

**Lemma 3.3.** For \( w \in L_2(I_n; [L_2(\Omega)]^3) \), \( \varphi \in L_2(I_n; [H_0^2(\Omega)]^3) \), \( \psi \in C(I_n; [H^1(\Omega)]^3) \), and \( \Phi \in W^2_{0n} \) constant in time, we have

\[
| \int_{I_n} \sum_{K \in T_n} \int_{\partial K \setminus \partial \Omega} w \cdot (\varphi - \Phi) \ ds \ dt | \\
\leq \int_{I_n} \sum_{K \in T_n} |w|_{\partial K \setminus \partial \Omega} \cdot \left( C^{k}_{n,K} k_n |\varphi|_{\partial K \setminus \partial \Omega} + C^{h}_{n,K} h^{3/2}_{n,K} |D^2 \varphi|_{K} \right) \ dt,
\]

where \( h_{n,K} \) is the diameter of element \( K \in T_n \), and \( D^2 \) measures second order derivatives with respect to \( x \).

**Proof.** We have

\[
| \int_{I_n} \sum_{K \in T_n} \int_{\partial K \setminus \partial \Omega} w \cdot (\varphi - \Phi) \ ds \ dt | \\
\leq | \int_{I_n} \sum_{K \in T_n} \int_{\partial K \setminus \partial \Omega} w \cdot (\varphi - \bar{\varphi}) \ ds \ dt | + | \int_{I_n} \sum_{K \in T_n} \int_{\partial K \setminus \partial \Omega} w \cdot (\bar{\varphi} - \Phi) \ ds \ dt | = I_1 + I_2.
\]

For \( I_1 \) we use the Cauchy-Schwarz inequality for each element, then (3.5), to get

\[
I_1 \leq \int_{I_n} \sum_{K \in T_n} |w|_{\partial K \setminus \partial \Omega} \cdot \left( C^{k}_{n,K} k_n \sup_{\eta \in I_n} |\varphi(\eta)|_{\partial K \setminus \partial \Omega} \right) \ dt.
\]

\( I_2 \) is estimated by the Cauchy-Schwarz inequality for each element, and the standard interpolation estimate \( \|h^{-3/2}_{n,K}(\bar{\varphi} - \Phi)\|_{\partial K \setminus \partial \Omega} \leq C\|D^2 \varphi\|_K \), for each \( t \in I_n \), to get

\[
I_2 \leq \int_{I_n} \sum_{K \in T_n} |w|_{\partial K \setminus \partial \Omega} \cdot \left( C^{h}_{n,K} h^{3/2}_{n,K} |D^2 \varphi|_{K} \right).
\]

**Theorem 3.4** (A posteriori error estimate for the cG(1) method). If \( u^h \) solves (2.3), \( (U_h, P_h) \) solves (2.7) with \( \delta_1 = \delta_2 = 0 \), \( (\varphi, \theta) \) solves (3.2), and \( \psi \in L_2(I; [L_2(\Omega)]^3) \) is given, then

\[
| \int_Q (u^h - U_h) \cdot \psi \ dx \ dt | \leq e_D + e_M,
\]

where \( e_D \) is a discretization error and \( e_M \) a modeling error, defined by

\[
e_D = \sum_{n=1}^N \left\{ \int_{I_n} \sum_{K \in T_n} |R_1(U_h, P_h)|_K \cdot \omega_1 \ dt + \int_{I_n} \sum_{K \in T_n} |R_2(U_h)|_K \cdot \omega_2 \ dt \\
+ \int_{I_n} \sum_{K \in T_n} R_3(U_h) \cdot \omega_3 \ dt \right\}
\]

\[
e_M = \sum_{n=1}^N \left\{ \int_{I_n} \sum_{K \in T_n} |R_4(u, U_h)|_K \cdot \omega_4 + R_5(U_h) \cdot \omega_5 \ dt \right\}
\]
with the residuals

\[ R_1(U_h, P_h) = \dot{U}_h + (U_h \cdot \nabla)U_h + \nabla P_h - \nu \Delta U_h + \nabla \cdot \dot{\tau}^h(U_h) - f^h, \]

\[ R_2(U_h) = \nabla \cdot U_h, \]

\[ R_3(U_h) = \frac{1}{2} h_{n,K}^{-1/2} \sup_{S \subset \partial K} \left( \left| \left( \nu \nabla U_h - \dot{\tau}^h(U_h) \right) \cdot n_S \right|, \left| \left( \nu \nabla U_h - \dot{\tau}^h(U_h) \right)_3 \cdot n_S \right| \right), \]

\[ R_4(u, U_h) = \nabla \cdot (\tau^h(u) - \dot{\tau}^h(U_h)), \]

\[ R_5(U_h) = \frac{1}{2} \sup_{S \subset \partial K} \left( \left| (\tau^h(U_h))_1 \cdot n_S \right|, \left| (\tau^h(U_h))_3 \cdot n_S \right| \right), \]

where \((M)_i\) denotes the \(i\)th row of the matrix \(M\), and the dual weights

\[ \omega_1 = C_{n,K}^k k_n |\dot{\varphi}|_{K,\infty} + C_{n,K}^h h_{n,K}^2 |D^2 \varphi|_K, \]

\[ \omega_2 = C_{n,K}^h k_n |\varphi|_{K,\infty} + C_{n,K}^h h_{n,K}^2 |D^2 \theta|_K, \]

\[ \omega_3 = C_{n,K}^h k_{n}^{1/2} |\dot{\varphi}|_{\partial K \setminus \partial \Omega, \infty} + C_{n,K}^h h_{n,K}^2 |D^2 \varphi|_K, \]

\[ \omega_4 = |\varphi|_K, \]

\[ \omega_5 = |\varphi|_{\partial K \setminus \partial \Omega, \infty}, \]

where \(h_{n,K}\) is the diameter of element \(K \in T_n\), \(D^2\) measures second order derivatives with respect to \(x\), and \(C_{n,K}^k, C_{n,K}^h\) represent interpolation constants.

Proof. Using Lemma 3.1, the continuity in time of the trial functions in (2.7), and the Galerkin orthogonality of (2.7), assuming \(\delta_1 = \delta_2 = 0\), to subtract interpolants \((\Phi, \Theta) \in W_{0n}^3 \times W_n\) that are piecewise constant in time over \(I_n\), we get

\[
\begin{align*}
| \int_Q (u^h - U_h) \cdot \psi \, dx \, dt | &= | \sum_{n=1}^{N} \left\{ (P_h - \dot{U}_h + (U_h \cdot \nabla)U_h, \varphi - \Phi)_n + (\dot{\tau}^h(U_h) - \nu \nabla U_h, \nabla (\varphi - \Phi))_n \\
&\quad + (P_h, \nabla \cdot (\varphi - \Phi))_n + (\nabla \cdot U_h, \theta - \Theta)_n + (\tau^h(u) - \dot{\tau}^h(U_h), \nabla \varphi)_n \right\}. 
\end{align*}
\]

Integration by parts in the viscous term results in non zero boundary integrals over interior element boundaries \(\partial K \setminus \partial \Omega\), for each \(t\), since \(\nabla U\) is piecewise constant in \(x\) over the elements, and thus discontinuous over interior element boundaries, and we have the same problem for the pressure term since the pressure is continuous in \(x\) over element boundaries, and so is \(\varphi - \Phi\) and \(\tau^h(u)\).

To estimate these element boundary integrals we use a standard finite element technique, see e.g. [12], where we first rewrite the sum of interior element boundary integrals as a sum of jumps of the form \(|\nu \nabla U_h \cdot n_S|\) in normal derivative over all interior faces \(S\) in \(T_n\), with \(n_S\) being a globally defined unit normal vector associated with the face \(S\). We then attribute half of the jump to each of the two elements.
sharing the face and rewrite the sum again over the elements $K \in T_n$, to get

$$
| \int_Q (u^h - U_h) \cdot \phi \, dx \, dt |
$$

$$
\leq \sum_{n=1}^N \{ |(\hat{U}_h + (U_h \cdot \nabla)U_h + \nabla P_h - \nu \Delta U_h + \nabla \cdot \hat{\tau}^h(U_h) - f^h, \varphi - \Phi)_n |
$$

$$
+ |(\nabla \cdot U_h, \theta - \Theta)_n | + \int_{I_n} \sum_{K \in T_n} \int_{\partial K \setminus \partial \Omega} \frac{1}{2} [ (\nu \nabla U_h - \hat{\tau}^h(U_h)) \cdot n_S ] \cdot (\varphi - \Phi) \, ds \, dt |
$$

$$
+ |(\nabla \cdot (\tau^h(u) - \hat{\tau}^h(U_h)), \varphi)_n | + \int_{I_n} \sum_{K \in T_n} \int_{\partial K \setminus \partial \Omega} \frac{1}{2} [ \hat{\tau}^h(U_h) \cdot n_S ] \varphi \, ds \, dt \}.
$$

We use Cauchy-Schwarz inequality for each element, and Lemma 3.2 and Lemma 3.3 are then used to estimate the interpolation errors.

We note that the modeling error $e_M$ contains $\tau^h(u)$, which depends on $u$, the unknown solution to the Navier-Stokes equations. This means that strictly speaking Theorem 3.4 is not an a posteriori error estimate. In the computational examples in this paper we use a scale similarity subgrid model [36] to estimate $\tau^h(u)$. Further, in this paper we use the stabilization as a subgrid model, and thus $\hat{\tau}^h(U_h) = 0$ in the computational examples.

Although, a very important point is here that to use Theorem 3.4 to estimate the error in a chosen output quantity we do not need to estimate $\tau^h(u)$ itself, but only the size of $\tau^h(u)$ acting on the dual solution. For example, if the dual solution is smooth, the action of $\tau^h(u)$ on this dual solution may be very small even though $\tau^h(u)$ in itself is large.

This crucial observation explains why it may be cheap to compute global output quantities such as mean values in a turbulent flow, while pointwise output quantities may be very expensive. Global output leads to smooth data to the dual problem, and thus typically regular solutions, while pointwise output quantities leads to irregular data to the dual problem. In a continuation of this paper [26] the action of $\tau^h(u)$ on the dual solution is estimated directly, without first estimating $\tau^h(u)$.

### 3.3. Remarks on the linearization error in the dual problem

The a posteriori error estimate in Theorem 3.4 is constructed to be useful in an adaptive algorithm as a stopping criterion, a refinement criterion for the space and time discretization, and an error indicator for the subgrid model. See e.g. [22] for applications of this type of a posteriori error estimates to laminar flow in 3d for the computation of linear functionals in benchmark problems.

To evaluate the error bounds in Theorem 3.4, we approximate the dual weights $\omega_i$ numerically, by computing approximate solutions to the dual problem (3.2). In the computation of the dual problem (3.2) we do not have access to $u^h$, the solution to (2.3). Instead we approximate $u^h$ by $U_h$, a finite element approximation of $u^h$, which thus introduces a linearization error $u^h - U_h$ in the dual problem.

In this paper we make the assumption that in an adaptive algorithm driven by Theorem 3.4, $U_h$ converges to $u^h$ pointwise, and that thus the linearization error converges pointwise to zero. Such an assumption gives some justification for using Theorem 3.4 in an adaptive algorithm, although there may still be problems when the computational mesh is not fine enough, and/or the subgrid model is not a sufficiently good approximation of the Reynolds stresses.
Practical experience from using this type of a posteriori error estimates for adaptive mesh refinement for various problems has been positive, with effective mesh refinement criterions and sharp a posteriori error estimates, see e.g. [22, 6] for examples for incompressible flow.

Alternative forms of the linearized dual problem (3.2) are possible. For example, the dual problem may be linearized at $u$, the exact solution of (2.1), but then the corresponding linearization error $u - U_h$ in the dual problem can never be pointwise small in a LES (by definition we do not resolve all scales in a LES). Typically the error $u - U_h$ is large pointwise, since $u$ contains finer scales than $U_h$. The effect of the linearization error is still not fully understood.

4. Numerical results. In [25] a computational study of transition to turbulence in shear flow is conducted from which we estimate the error in a turbulent Couette flow for $Re = \nu^{-1} = 10000$, using Theorem 3.4. In particular, we solve the associated time dependent linearized dual Navier-Stokes equations in 3d for various data corresponding to estimates of the error in different linear functionals of the solution to the averaged Navier-Stokes equations (2.3). In the computations the cG(1)cG(1)-method (2.7) is used, see e.g. [29] for other examples where stabilized finite element methods are used for turbulence simulation. We do not use any other subgrid model than the numerical stabilization, which is referred to as the no model approach in [36]. We compute on the unit cube with a regular tetrahedral mesh with $65 \times 65 \times 65$ nodes. Periodic boundary conditions were used in the streamwise $x_1$-direction and in the spanwise $x_3$-direction, and on top and bottom the streamwise velocity is $\pm 1$.

4.1. Computation of the dual problem. In the computations of the dual problem we use a cG(1)cG(1)-method, corresponding to the method used for the primal problem, on a regular tetrahedral mesh with $33 \times 33 \times 33$ nodes. Both $u^h$ and $U_h$ in (3.2) are approximated by $U_h$, projected onto this mesh. In this paper we have sampled $U_h$ at 41 points in time over a time interval of length 10, and we have used linear interpolation in time for intermediate values.

Compared to the primal problem, the dual problem is linear and thus typically cheaper to solve. In this paper the cost of computing the dual problem is roughly about 10% compared to the cost of computing the primal problem.

4.2. Discretization error vs. modeling error. We now use Theorem 3.4 to estimate the error in the computation of the turbulent flow described above. We consider the time interval [20, 30], where we have a fully developed turbulent flow, see [25], and we assume that the initial condition from $t = 20$ is exact. From Theorem 3.4, we have that

$$|\int_Q (u^h - U_h) \cdot \psi \, dx \, dt| \leq e_D + e_M,$$

where $e_D$ represents a discretization error and $e_M$ represents a modeling error. Here we set $h = 1/64$ in the definition of $u^h$, which corresponds to the size of the uniform computational mesh. The Reynolds number $Re = \nu^{-1} = 10000$, so we expect that the underlying exact flow contains finer scales than $h$ for fully developed turbulence, according to standard Kolmogorov theory [15].

For both the discretization error and the modeling error we need to approximate the dual solution $(\varphi, \theta)$ numerically. The discretization residuals are directly computable from the approximate solutions $(U_h, P_h)$, whereas the modeling residual $R_M(u, U_h)$ has to be estimated. In the estimation of the discretization error we use
$C_{n,K}^h = 1/8$ and $C_{n,K}^k = 1/2$, which are approximations of the interpolation constants motivated by a simple calculation on a reference element.

We note that there are many different ways to estimate the dual weights. Instead of using interpolation error estimates in terms of higher derivatives of the dual solution, we may, for example, try to estimate the interpolation error by various approximations on coarser meshes.

We use the following scale similarity subgrid model from [33] to estimate the modeling residual $R_M(u,U_h) = \nabla \cdot \tau^h(u)$:

$$\tau^h_i(u) \approx C_L \tau^{H}_{ij}(u^h) = C_L((u^h_i u^h_j)^H - (u^h_i)^H(u^h_j)^H), \quad (4.1)$$

with $C_L = 1$ and $H > h$. In the computations we approximate $u^h$ by $U_h$.

In the computations we use the numerical stabilization as the only subgrid model, which is referred to as the no model approach in [36], and thus $\tilde{\tau}^h(U_h) = 0$.

**Remark 4.1.** To construct the computational mesh $\mathcal{T}_n$, we start from a regular subdivision of the unit cube into 6 tetrahedrons. We then successively, for each refinement level, divide the tetrahedrons into 8 new tetrahedrons, so that each level of refinement corresponds to a regular subdivision of the unit cube into subcubes with half the side length of the preceding level, which is then divided into 6 tetrahedrons. We approximate the spatial filter operation on $H$ in (4.1) by projection onto the finite element space of continuous piecewise linear polynomials on a coarser tetrahedral mesh, with side length $H = 2h = 2 \times 1/64 = 1/32$ in the corresponding mesh of cubes.

**4.3. Computation of space-time averages.** In this section we estimate the error in various space-time averages $g(u^h)$ of the filtered velocity field $u^h$, of the form (3.1), with

$$\psi = (\chi_{\omega \times [30,d(\omega),30]} / |\chi_{\omega \times [30,d(\omega),30]}|, 0, 0), \quad (4.2)$$

where $\chi_D$ is the characteristic function for $D \subset \Omega \times I$, and $|D|$ denotes the space-time volume of $D$. That is, we are interested in the error in an average of $u^h_i$ over the space-time domain $\omega \times [30-d(\omega),30]$, with $\omega$ being a spatial cube with side length $d(\omega)$ centered at $(0.5,0.5,0.5)$, corresponding to a space-time cube with side length $d(\omega)$ centered at $(x,t) = (0.5,0.5,0.5,30-d(\omega)/2)$.

The dual problems are solved backwards in time, and we find that although data from the spatial cube $\omega$ is spread throughout the computational domain by the convective, diffusive, and reactive mechanisms of the dual equation (3.2), the dual solution does not grow exponentially as predicted by worst case analytical estimates.

In Figure 4.1 we present the computationally approximated a posteriori error bounds of the discretization error $e_D$ and the modelling error $e_M$, for the error in the functional (3.1) with data from (4.2). Figure 4.1 should be understood as the errors for different starting times in $[20,30]$, assuming that the solution at these starting times is exact.

We find that the estimates of $e_D$ and $e_M$ are of the same order in this computation, and both errors of course increase if we compute over a longer time. We note that, in this example, both $e_D$ and $e_M$ are larger for smaller space-time averages.

Theorem 3.4 says that the error can be estimated by space-time integrals of residuals multiplied by dual weights. The residuals measure how well the computed solution satisfies the differential equation pointwise, and the dual weights determine how the residuals influence the particular error measure considered.
Fig. 4.1. $e_D$ (‘-’) and $e_M$ (‘*’) for $d(\omega) = 0.125$ (upper), 0.25 (middle), 0.5 (lower), as functions of time.
The size of the residuals in the computation for \( t \in [20, 30] \) is fairly constant in time, whereas the solution of the dual problem grows (backwards) in time. In Figure 4.2 we plot the \( L_1 \)-norms of the dual solutions for \( d(\omega) = 0.5, 0.25, 0.125 \). In the initial phase (for backward time) the dual solutions grow through the action of the source term \( \psi \) over the time interval \([30 - d(\omega), 30]\), and this initial growth is larger for smaller \( d(\omega) \).

**Fig. 4.2.** \( \|\varphi\|_1 \) for \( d(\omega) = 0.5, 0.25, 0.125 \) linearized at a turbulent flow (left), and a time average over \( \omega \times [20, 30] \) for a turbulent flow (right), as functions of time.

In the next phase, for \( t < 30 - d(\omega) \), when the source term \( \psi \) is zero, there is a growth in the dual solution due to the reaction term \( \nabla U_h \cdot \varphi \) in (3.2), which is connected to the irregularity of the computed solution \( U_h \). When the dual solution is spread over a larger part of the domain, by convective and diffusive mechanisms, this growth is weakened by cancelations, which is also the reason why the growth is weaker for larger \( d(\omega) \).

The results in this example support the intuitive idea that larger space-time averages are less computationally demanding than small, which implies that we may, for example, be able to compute an approximation of a time average of a certain quantity with a small error to an acceptable computational cost, even though it may be computationally very expensive to approximate this quantity at a specific time. For the error in space-time averages of the solution over \( \omega \times [20, 30] \), the \( L_1 \)-norm of the dual solutions for various \( d(\omega) \) are plotted in Figure 4.2, where now the source term \( \psi \) is active over the whole time interval in the solution of the dual problem. We find that in this case the dual solution is smaller than in the previous examples, with smaller time averages, as expected.

**Remark 4.2.** In the estimate of the discretization error we have neglected the residual \( R_2(U_h) \), since the other residuals dominate for \( \nu \) small.

**4.4. Stability properties of laminar vs. turbulent flow.** In Figure 4.3 we plot the \( L_1 \)-norm of the dual solution linearized at the laminar Couette flow \( u = (2(y - 0.5), 0, 0) \), with \( Re = \nu^{-1} = 100 \), where we have no growth from the reaction term, since diffusive mechanisms dominate. Instead the dual solution is quickly damped followed by a slow further decrease caused by diffusive mechanisms.

In Figure 4.3 we then plot the case of the dual solution linearized at the same laminar flow, but now for \( Re = \nu^{-1} = 10000 \), which corresponds to a highly unstable laminar flow. In this case we get an initial growth of the dual solution due to the reaction term in (3.2), since the diffusive mechanisms are weaker, after which we
Fig. 4.3. $\|\varphi\|_1$ for $d(\omega) = 0.5, 0.25, 0.125$ linearized at a laminar flow with $Re = \nu^{-1} = 100$ (left), and a laminar flow with $Re = \nu^{-1} = 10000$ (right), as functions of time.

get a similar scenario as in the case of $Re = \nu^{-1} = 100$. That is, in this example it is more computationally demanding to compute a numerical approximation of the unstable laminar flow with a larger Reynolds number, even though the exact solution is the same in both cases.

**Remark 4.3.** The computations of the linearized dual problems in this paper were all performed with various characteristic functions as data, without the scaling corresponding to the space-time volume of the domain over which the data acted. The solutions were then postprocessed to obtain the proper scaling. This procedure was unfortunate since the relative numerical errors were amplified in the computations for small space-time averages, leading to the wiggles in the graphs in Figure 4.2 and Figure 4.3. We accept the computations here since we are mainly interested in the qualitative properties of the dual solutions.

5. Conclusions and future directions. In this paper we investigated a posteriori error estimation for LES, using duality techniques, opening the possibility to extend adaptive finite element methods to LES, with adaptive choice of both discretization and subgrid model. The a posteriori error estimates bound the error in various norms with respect to the filtered velocity, as well as the error in linear functionals of the filtered velocity, in terms of a space-time integral of discretization residuals and modeling residuals multiplied by dual weights. The dual weights are obtained from computational approximation of associated linearized dual problems. The discretization residual is directly computable from the approximate solution, and the modeling residual needs to be estimated. In this paper we used a scale similarity subgrid model to estimate the modeling residual. The extension to a posteriori error estimation involving the pressure, or surface integrals, such as drag or lift forces, is straightforward, using the techniques in [22].

We evaluated the a posteriori error estimates in the case of transition to turbulence in Couette flow, solving the corresponding time dependent linearized dual Navier-Stokes equations in 3d numerically for various data, corresponding to a posteriori error estimates of different output functionals of the filtered velocity field. These computations provided qualitative results for the considered flow example, such as support for the intuitive ideas that the computation of small averages of the velocity is more computationally demanding than larger averages, and that turbulent flow is more computationally demanding than laminar. In particular, we note that the dual
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solutions does not explode, but stay bounded, indicating computability of certain mean quantities in the turbulent flow considered in this paper.

In continuations of this work we use these a posteriori error estimates in an adaptive finite element method for LES [21], and in [26] we extend to Adaptive DNS/LES.

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REFERENCES


