A New Approach to Computational Turbulence Modeling

J. Hoffman and C. Johnson

Abstract

We present a new approach to Computational Fluid Dynamics CFD using adaptive stabilized Galerkin finite element methods with duality based a posteriori error control for chosen output quantities of interest. We address the basic question of computability in CFD: For a given flow, what quantity is computable to what tolerance to what cost? We focus on incompressible Newtonian flow with medium to large Reynolds numbers involving both laminar and turbulent flow features. We estimate a posteriori the output of the computed solution with the output based on the exact solution to the Navier-Stokes equations, thus circumventing introducing and modeling Reynolds stresses in averaged Navier-Stokes equations. Our basic tool is a representation formula for the error in the quantity of interest in terms of a space-time integral of the residual of a computed solution multiplied by weights related to derivatives of the solution of an associated dual problem with data connected to the output. We use the error representation formula to derive an a posterori error estimate combining residuals with computed dual weights, which is used for mesh adaptivity in space-time with the objective of satisfying a given error tolerance with minimal computational effort. We show in concrete examples that outputs such as mean values in time of drag and lift of turbulent flow around a bluff body are computable on a PC with a tolerance of a few percent using a few hundred thousand mesh points in space. We refer to our methodology as *Adaptive DNS/LES*, where automatically by adaptivity certain features of the flow are resolved in a *Direct Numerical Simulation DNS*, while certain other small scale turbulent features are left unresolved in a *Large Eddy Simulation LES*. The stabilization of the Galerkin method giving a weighted least square control of the residual acts as the subgrid model in the LES. The a posteriori error estimate takes into account both the error from discretization and the error from the subgrid model. We pay particular attention to the stability of the dual solution from (i) perturbations replacing the exact convection velocity by a computed velocity, and (ii) computational solution of the dual problem, which are the crucial aspects entering by avoiding using averaged Navier-Stokes equations including Reynolds stresses. A crucial observation is that the contribution from subgrid modeling in the a posteriori error estimation is small, making it possible to simulate aspects of turbulent flow without accurate modeling of Reynolds stresses.

Key words: adaptivity, computability, adaptive finite element method, a posteriori error estimate, turbulence, incompressible flow, DNS, LES
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1 Introduction

The outstanding open problem of fluid dynamics, since Reynolds pioneering work in the late 19th century, is *turbulence modeling*, or the simulation of turbulence using mathematical models. The *Reynolds number* $Re = \frac{UL}{\nu}$, where U is a characteristic flow velocity, L a characteristic length scale, and ν the viscosity of the fluid, may be used to characterize different flow regimes. If Re is relatively small ($Re \leq 10 - 100$), then the flow is viscous and the flow field is ordered and smooth or *laminar*, while for larger Re, the flow will at least partly be *turbulent* with time-dependent non-ordered features on a range of length scales down to a smallest scale of size $Re^{-3/4}$, assuming $L = 1$. In many applications of scientific and industrial importance Re is very large, of the order 10^6 or larger, and the flow shows a combination of laminar and turbulent features.

The Navier-Stokes equations formulated in 1825-45 appear to give an accurate description of fluid flow including both laminar and turbulent flow features. *Computational Fluid Dynamics CFD* concerns the computational simulation of fluid flow by solving the Navier-Stokes equations numerically. CFD has developed quickly with the rapid growth of desk-top computing power, and one might expect that today the problem of turbulence modeling can been solved by CFD. The turbulence modeling would then be achieved simply by computing solutions to the Navier-Stokes equations including computing turbulent flow. However, to computationally resolve all the features of a flow at $Re = 10^6$ in such a *Direct Numerical Simulation DNS* would require of the order $Re^3 = 10^{18}$ uniformly distributed mesh points in space-time, and thus would be impossible on any forseeable computer, and of course was impossible for Reynolds.

To get around the impossibility of DNS at higher Reynolds numbers various techniques of turbulence modeling have been attempted since the days of Reynolds. All these techniques are based on some kind of *averaging*, where one seeks to solve modified Navier-Stokes equations which would be satisfied by certain averages of the true solution. The averages may be global in space/time or statistical ensemble averages, leading to *RANS* models, or more local in space-time in *Large Eddy Simulation LES* with the coarser scales being resolved computationally. The basic idea would thus be to find modified Navier-Stokes equations for certain averages which could be computationally solved, instead of the seemingly unsolvable true Navier-Stokes equations. Such modified or averaged Navier-Stokes equations always contain so called *Reynolds stresses* resulting from the averaging of nonlinear terms, which have the form of generalized covariances. The turbulence modeling would then boil down to modeling of the Reynolds stresses. In a LES one would this way attempt to model the influence of the unresolved small scales on the resolved larger scales in a *subgrid model*. Many subgrid models have been proposed, but no clear answer to the question of the feasibility of LES in simulation of turbulence has been given. In fact, the nature of the Reynolds stresses have remained largely a mystery, with little progress in their modeling. A main open problem of CFD today is the simulation of laminar/turbulent flow at high Reynolds numbers by some form of LES.

In this note we take a fresh look at computational turbulence modeling and LES, with focus on incompressible Newtonian flow governed by the incompressible Navier-Stokes equations. We shall present evidence that we may computationally approach the true Navier-Stokes equations (without any Reynolds stresses to model), and that this way it is possible to compute certain aspects of turbulent flow without resolving all the flow features in a DNS. This is analogous to the observed fact that we may compute certain aspects of a shock problem for compressible flow without resolving shocks to their actual physical width. We thus circumvent the whole procedure of attempting to solve some form of averaged Navier-Stokes equations including the modeling of Reynolds stresses.

Our new approach to computational turbulence modeling may be viewed as an application of the general methodology of adaptive stabilized Galerkin finite element methods with duality-based a posteriori error control for chosen output quantities of interest, developed in [5,14,10,8,9,15,16,12,13]. Our basic tool underlying the a posteriori error estimate is a representation of the error in output in terms of a space-time integral of the residual of a computed solution multiplied by weights related to derivatives of the solution of an associated dual linearized problem with data connected to the output. We use an adaptive procedure where we compute on a sequence of successively refined meshes with the objective of reaching a stopping criterion based on the a posteriori error estimate with minimal computational effort (minimal number of mesh points in space-time). We show in concrete examples that outputs such as a mean value in time of the drag of a bluff body in a laminar/turbulent flow is computable on a PC (with tolerances on the level of a few percent using a few hundred thousand mesh points in space).

The stabilized Galerkin method is the Galerkin/least squares space-time finite element method developed over the years together with Hughes, Tezduyar and coworkers, here referred to as the General Galerkin G^2-method. This method includes the *streamline diffusion method* on Eulerian space-time meshes, the *characteristic Galerkin method* on Lagrangian space-time meshes with orientation along particle trajectories, and *Arbitrary Lagrangian-Eulerian ALE methods* with different mesh orientation. G^2 offers a general flexible methodology for the discretization of the incompressible and compressible Navier-Stokes equations applicable to a great variety of flow problems from creeping low Reynolds number flow through medium to large Reynolds number turbulent flow, including free or moving boundaries. With continuous piecewise polynomials in space of order p and discontinuous or continuous piecewise polynomials in time of order q, we refer to this method as cG(p)dG(q) or cG(p)cG(q). Below we present computational results with cG(1)cG(1).

We describe the methodology for CFD presented in these notes as *Adaptive DNS/LES*

G^2, where automatically by adaptivity certain features of the flow are pointwise resolved in a DNS, while certain other small scale features are left unresolved in a LES. The stabilization in G^2 (adding a weighted least square control of the residual) acts as a subgrid model in LES introducing viscous damping of high frequencies. The G^2 subgrid model is similar to a standard Smagorinsky model (adding a viscous term with viscosity proportional to $h^2|\epsilon(U_h)|$, where $h = h(x)$ is the local mesh size in space, U_h the discrete computed solution, and $\epsilon(U_h)$ the strain tensor), but with less damping of low frequencies.

The a posteriori error estimate underlying the stopping criterion has (i) a contribution from the residual of the Galerkin solution inserted in the true Navier-Stokes equations (which estimates the output error from the Galerkin discretization) and (ii) a contribution from the stabilization (which estimates the output error from the subgrid model). If we reach the stopping criterion, this means that the sum of (i) and (ii) are below the tolerance, and thus in particular that the contribution from the subgrid model to the output error is below the tolerance.

The G^2 subgrid model may be viewed as adding a viscosity roughly of size $h(x)$ in areas of turbulence, and thus G^2 will act as a LES if $h(x) > \nu$ in a turbulent area. We will show below that the mean drag of a bluff body in a benchmark problem at Reynolds number 40.000, with $\nu = 2.5 \times 10^{-5}$, is computable up to a tolerance of a few percent with $h(x) \approx 10^{-2}$ (thus $h(x) >> \nu$) in the turbulent wake, thus definitely using LES in part of the domain.

We thus show that certain outputs of a partly turbulent flow are computable without resolving all the small scale features of the turbulent flow by using a relatively simple subgrid model. The reason this is possible is that the output does not depend on all the exact details of the turbulent flow, which we observe by computing the contribution to the a posterori error estimate from the subgrid model and noting that this contribution indeed is small. As indicated, this is analogous to the observed fact that in a shock problem for compressible flow, certain outputs are computable without resolving the shocks to their actual width.

The fact that certain outputs do not critically depend on the exact nature of the subgrid model being used, does not mean that we can do without a subgrid model. The local intensity of dissipation in a turbulent flow is a characteristic feature of the flow which has to be captured in the subgrid model to its correct level, but certain outputs may be insensitive to the exact nature of the dissipation. More precisely, the dissipation in LES may occur at coarser scales than in the real flow, while the total dissipation is correct. In [12], we notice this phenomenon for a bluff body problem, where the intensity of the dissipation in the turbulent wake is nearly constant during the refinement process (captured in a LES), while the volume of the turbulent wake expands (captured in a DNS in the boundary layer surrounding the wake), until the correct volume is captured.

The key test of computability in Adaptive DNS/LES G^2 of a certain output is thus the a posteriori error estimate combining residuals with dual weights. If indeed this combination is small enough, which we test computationally, then we reach the stopping criterion and thus we have computed the desired output to the given tolerance. Evidently, the size of the dual weights are here crucial: if the weights are too large, then we may not be able to reach the stopping criterion with available computing power. We observe that large mean value outputs such as the time average of drag and lift typically have smaller dual weights than more pointwise outputs. Altogether, we may say that the computability of a certain output directly couples to the size of the dual weights and thus by computing these weights the computability of a certain output can be assessed.

The dual problem is a linear convection-diffusion-reaction problem with the gradient ∇U_h acting as the coefficient in the reaction term, and the exact flow velocity u acting as the convection coefficient. In turbulent flow ∇U_h will be large, and thus potentially generating exponential growth of the dual solution and very large dual weights. Nevertheless, the dual solution and the dual weights turn out to be of moderate size, which we observe by computing the dual solution, and which we intuitively may explain by the fact that ∇U_h is fluctuating with a combination of production and consumption in the reaction, with apparently only a moderate net production. This is the crucial fact behind the computability of certain output, which we may view as a fortunate "miracle" of CFD, and which may be very difficult to "understand" or rationalize by mathematical analysis, although we may successively get used to it by computing dual solutions and eventually possibly grasping it intuitively.

To compute the crucial dual problem we have to replace the unknown u by the a computed U_h, and we thus have to deal with the corresponding perturbation of the dual solution. We give computational evidence that the features of the dual solution entering into the a posteriori error estimate, are reasonably stable under such a perturbation.

The key new ingredient in our work as presented in these notes is the use of duality to assess the basic problem of computability of a specific output for a specific flow. In particular, we show that the crucial dual solution may be computed at an affordable cost for complex time-dependent laminar/turbulent flows in 3d.

We may view the stabilized Galerkin method as producing an approximate solution of the Navier Stokes equations, with a residual which in a weak sense is small (reflecting the Galerkin orthogonality) and which is also controlled in a strong sense (reflecting the least squares stabilization). The existence and uniqueness of exact solutions to the Navier-Stokes equations is one of the major open problems of mathematical analysis today, as formulated one of the ten $1 million Clay Prize problems. It is conceivable that new input to this problem may come from computed solutions with a posteriori error control. In particular, the dual weights carry sensitivity information which directly relates to the question of uniqueness, investigated in [17].

We emphasize the following key aspects of the new approach:

1.1 Comparing the outputs of u and U_h without using Reynolds stresses

We get around introducing any Reynolds stresses by directly comparing the output of the exact solution u with the output of the computed solution U_h. We thus do not compare with the output of an average u^h of u, which would introduce Reynolds stresses. Indeed, if the output is an average, then it seems natural to directly compare the output of u and U_h, since this anyway would boil down to comparing some kind of average of u (output of u) with that of U_h. Introducing the output of an average u^h would seem to correspond to unnecessarily averaging twice.

Circumventing using Reynolds stresses may potentially bring substantial simplifications to CFD. Countless articles have addressed the open problem of modeling Reynolds stresses, without any clear results coming out, except possibly many observations that simple Smagorinsky models may in fact in many cases give reasonable results. A major difficulty in CFD has been the lack of a posteriori error estimation allowing objective comparison of different models. With a posteriori error estimation now available, it is possible to compare models and in particular show that simple models may suffice.

The Reynolds stresses are fictitious quantities without clear physical meaning which are difficult to measure, and thus also to model. In particular, an aspect of *backscattering* representing effects on large scales from small scales has presented seemingly unsurmounatble problems of modeling. Our experience indicates that such effects may be small on certain outputs, and thus that a dissipative subgrid model may be enough.

1.2 The stability of the dual solution under perturbations

Comparing directly the output of u and U_h, we have to live with the fact that U_h may not be a pointwise approximation of u. The error representation survives this fact, but we have to deal with a dual linear problem with the convection velocity being the exact velocity u. In practice we replace u by a computed U_h and the crucial question is then the effect of this (pointwise possibly large) perturbation on the dual solution, or rather the aspects of the dual solution appearing in the a posteriori error estimate. We give computational evidence that these aspects may be quite stable also under the perturbation, and thus that the effect of the perturbation may be small. Intuitively, u is fluctuating around U_h and thus their net effect by convection on the dual solution may be quite similar.

We thus circumvent having to introduce Reynolds stresses by directly estimating the outputs of u and U_h a posteriori, and the crucial feature is then the stability of the dual solution under the perturbation from (i) changing the true convection velocity from u to U_h (as we just discussed), and (ii) solving the dual problem computationally. We give evidence that the dual solution is indeed sufficiently stable under (i) and (ii), and in doing so we in particular use the fact that the effect on output of the stabilization acting as subgrid model, indeed comes out as being small. We could take this as evidence that also the effect of the true Reynolds stresses (if we decided to anyway work with an averaged model) would be small, and thus that a crude Reynolds stress model might indeed work. But as we said, we see no real need to consider averaged Navier-Stokes equations with associated Reynolds stresses.

We have thus reformulated the basic problem of turbulence modeling using Reynolds stresses to a question of a certain stability aspects of dual solutions, which we can seek to answer by computation. The key to success in this reformulation is the fact that the modeling error is indeed small. In Adaptive DNS/LES we continue the refinement until the modeling error is small. We observe in computations of e.g. drag that we may reach the stopping criterion with only about 10^5 mesh points in space, thus effectively using LES in large volumes of turbulent flow.

1.3 On the standard small perturbation approach

In the standard approach to duality-based a posteriori error estimation, we view the dual problem as a *linearized* problem derived under a small perturbation assumption that the computed solution is a pointwise approximation of the true solution. However, the error representation can be set up also in the case of large perturbations, which opens a wide area of applications, including turbulence modeling. As indicated the crucial question is now the stability of the dual solution under perturbations.

1.4 Artificial viscosity

We have indicated that the effective subgrid model resulting from the stabilized Galerkin method, may be viewed as a non-standard Smagorinsky model with dissipation mainly on the smallest computational scales. We thus use a kind of so called *artificial viscosity*, similar to that being used in shock problems for compressible flow. We observe that certain outputs of a turbulent flow may be computed with artificial viscosity methods, just as certain outputs in a shock problem may be computed using such methods.

2 References

For an overview of adaptive finite element methods including references, we refer to the survey articles [5], [4], and the books [6], and [2], containing many details on various aspects of adaptive finite element methods omitted in these notes. For an overview of finite element methods for the incompressible Navier-Stokes equations including references, we refer to [20], and for an overview of computational methods for turbulence we refer to [21], and the references therein.

For incompressible flow, applications of adaptive finite element methods based on this framework have been increasingly advanced with computation of quantities of interest such as the drag force for 2d stationary benchmark problems in [3,7], and drag and lift forces and pressure differences for 3d stationary benchmark problems in [10]. In [14], time dependent problems in 3d are considered, and the extension of this framework to LES is investigated in [8,9]. This extension is crucial and opens for a large wealth of real world applications. The generalization to *Adaptive DNS/LES* is presented in [15,16,11,12,13], and in [17] results on *uniqueness in output* of weak solutions of the Navier-Stokes equations are presented.

3 The 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 Ω in $\mathbb{R}^3$ (where we assume that Ω is a polygonal domain) with homogeneous Dirichlet boundary conditions, take the form: Find (u, p) such that

$$\begin{aligned} \dot{u} + (u \cdot \nabla)u - \nu\Delta u + \nabla p = f \qquad & \text{in } \Omega \times I, \\ \nabla \cdot u = 0 \qquad & \text{in } \Omega \times I, \\ u = 0 \qquad & \text{on } \partial\Omega \times I, \\ u(\cdot, 0) = u_0 \qquad & \text{in } \Omega, \end{aligned} \tag{1}$$

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

$$\nu\Delta u - \nabla p = \text{div}\,\sigma(u,p), \tag{2}$$

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 δ_{ij} is the usual Kronecker delta, the indices i and j ranging from 1 to 3. We assume that (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 ν^{-1}.

4 Discretization: cG(1)cG(1)

The cG(1)cG(1) method is a variant of the G^2 method [18,16] 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. 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 linear functions on a mesh $\mathcal{T}_n = \{K\}$ of mesh size $h_n(x)$ with W^n_w the functions $v \in W^n$ satisfying the Dirichlet boundary condition $v|_{\Gamma_D} = w$.

We now seek functions (U_h, P_h), continuous piecewise linear in space and time, and cG(1)cG(1) for (1), with homogeneous Dirichlet boundary conditions, reads: For $n = 1, ..., N$, find $(U_h^n, P_h^n) \equiv (U_h(t_n), P_h(t_n))$ with $U_h^n \in V_0^n \equiv [W_0^n]^3$ and $P_h^n \in W^n$, such that

$$\begin{aligned}
&((U_h^n - U_h^{n-1})k_n^{-1} + \hat{U}_h^n \cdot \nabla \hat{U}_h^n, v) + (2\nu\epsilon(\hat{U}_h^n), \epsilon(v)) - (P_h^n, \nabla \cdot v) + (\nabla \cdot \hat{U}_h^n, q) \\
&+ (\delta_1(\hat{U}_h^n \cdot \nabla \hat{U}_h^n + \nabla P_h^n), \hat{U}_h^n \cdot \nabla v + \nabla q) + (\delta_2 \nabla \cdot \hat{U}_h^n, \nabla \cdot v) \\
&= (f, v + \delta_1(\hat{U}_h^n \cdot \nabla v + \nabla q)) \quad \forall (v,q) \in V_0^n \times W^n,
\end{aligned} \tag{3}$$

where $\hat{U}_h^n = \frac{1}{2}(U_h^n + U_h^{n-1})$, $\delta_1 = \frac{1}{2}(k_n^{-2} + |U|^2 h_n^{-2})^{-1/2}$ in the convection-dominated case $\nu < \hat{U}_h^n h_n$ and $\delta_1 = \kappa_1 h^2$ otherwise, $\delta_2 = \kappa_2 h$ if $\nu < \hat{U}_h^n h_n$ and $\delta_2 = \kappa_2 h^2$ otherwise, with κ_1 and κ_2 positive constants of unit size, and

$$(v, w) = \sum_{K \in \mathcal{T}_n} \int_K v \cdot w \, dx,$$

$$(\epsilon(v), \epsilon(w)) = \sum_{i,j=1}^{3} (\epsilon_{ij}(v), \epsilon_{ij}(w)).$$

We note that the viscous term $(2\nu\epsilon(U_h), \epsilon(v))$ may alternatively occur in the form $(\nu \nabla U_h, \nabla v) = \sum_{i=1}^3 (\nu \nabla (U_h)_i, \nabla v_i)$. In the case of Dirichlet boundary conditions the corresponding variational formulations are equivalent, but not so in the case of Neumann boundary conditions. If we have Neumann boundary conditions, we use the standard technique to apply these boundary conditions weakly.

In extreme situations with very large velocity gradients, we may add residual dependent *shock-capturing artificial viscosity*, replacing ν by $\hat{\nu} = \max(\nu, \kappa_3|R(U_h, P_h)|h^2)$, where $R(U_h, P_h) = \sum_{i=1}^{4} R_i(U_h, P_h)$ with

$$\begin{aligned} R_1(U_h, P_h) &= |\dot{U}_h + U_h \cdot \nabla U_h + \nabla P_h - f - \nu \Delta U_h|, \\ R_2(U_h, P_h) &= \nu D_2(U_h), \\ R_3(U_h, P_h) &= |\mathrm{div}\, U_h|, \end{aligned} \tag{4}$$

and where

$$D_2(U_h)(x,t) = \max_{y \in \partial K} (h_n(x))^{-1} |[\frac{\partial U_h}{\partial n}(y,t)]| \tag{5}$$

for $x \in K$, with $[\cdot]$ the jump across the element edge ∂K, and κ_3 is a positive constant of unit size. Note that $R_1(U_h, P_h)$ is defined elementwise and that with piecewise linears in space, the Laplacian ΔU_h is zero. In the computations presented below, we chose $\kappa_3 = 0$ corresponding to shutting off the artificial viscosity. Note that $R_1(U_h, P_h) + R_2(U_h, P_h)$ bounds the residual of the momentum equation, with the Laplacian term bounded by the second order difference quotient $D_2(U_h)$ arising from the jumps of normal derivatives across element boundaries.

5 Adaptive computation of the force on a bluff body

We want to compute a mean value in time of the force on a bluff body in a channel subject to a time-dependent turbulent flow:

$$N(\sigma(u,p)) \equiv \frac{1}{|I|} \int_I \int_{\Gamma_0} \sum_{i,j=1}^{3} \sigma_{ij}(u,p) n_j \phi_i \, ds \, dt, \tag{6}$$

where (u, p) solves (1) in the fluid volume Ω surrounding the body (using suitable boundary conditions as specified below), Γ_0 is the surface of the body in contact with the fluid, and ϕ is a unit vector in the direction of the force we want to compute, for example, ϕ directed along the channel in the direction of the mean flow corresponds to the drag force, and ϕ in a direction perpendicular to the mean flow corresponds to a lift force on the cube.We first derive an alternative expression for the force $N(\sigma(u,p))$, which naturally fits with a Galerkin formulation, by extending ϕ to a function Φ defined in the fluid volume Ω and being zero on the remaining boundary Γ_1 of the fluid volume. Multiplying the momentum equation in (1) by Φ and integrating by parts, we get using the zero boundary condition on Γ_1

$$\begin{aligned} N(\sigma(u,p)) = \frac{1}{|I|} \int_I & (\dot{u} + u \cdot \nabla u - f, \Phi) - (p, \nabla \cdot \Phi) \\ & + (2\nu\epsilon(u), \epsilon(\Phi)) + (\nabla \cdot u, \Theta) \, dt, \end{aligned} \tag{7}$$

where we also added the integral of $\nabla \cdot u = 0$ multiplied with a function Θ. Obviously, the representation does not depend on the particular extension Φ of ϕ, or Θ.

We are thus led to compute an approximation of the force $N(\sigma(u,p))$ from a computed (U_h, P_h) using the formula

$$\begin{aligned} N^h(\sigma(U_h,P_h)) = \frac{1}{|I|}\int_I (\dot{U}_h + U_h\cdot\nabla U_h - f, \Phi) - (P_h, \nabla\cdot\Phi) \\ +(2\nu\epsilon(U_h), \epsilon(\Phi)) + SD(\delta, U_h, P_h, \Phi, \Theta) + (\nabla\cdot U_h, \Theta)\, dt, \end{aligned} \tag{8}$$

where now Φ and Θ are finite element functions (with as before $\Phi = \phi$ on Γ_0 and $\Phi = 0$ on Γ_1), and where $\dot{U}_h = (U_h^n - U_h^{n-1})/k_n$ on I_n. By the Galerkin orthogonality (3), it follows that $N^h(\sigma(U_h, P_h))$ is independent of the choice of (Φ, Θ) (assuming for simplicity that we use Dirichlet boundary conditions).

5.1 The dual problem

We introduce the following linearized dual problem: Find (φ, θ) with $\varphi = \phi$ on Γ_0 and $\varphi = 0$ on Γ_1, such that

$$\begin{aligned} -\dot{\varphi} - (u\cdot\nabla)\varphi + \nabla U_h\cdot\varphi - \nu\Delta\varphi + \nabla\theta = 0 \qquad & \text{in } \Omega\times I, \\ \operatorname{div}\varphi = 0 \qquad & \text{in } \Omega\times I, \\ \varphi(\cdot, T) = 0 \qquad & \text{in } \Omega, \end{aligned} \tag{9}$$

where $(\nabla U_h \cdot \varphi)_j = (U_h)_{,j}\cdot\varphi$. We notice that the dual problem is a linear convection-diffusion-reaction problem where the convection acts backward in time and in the opposite direction of the exact flow velocity u. We further note that the coefficient ∇U_h of the reaction term locally is large in turbulent regions, and thus potentially generating rapid exponential growth. However, ∇U_h is fluctuating and the net effect of the reaction term turns out to generate slower growth, as we learn from computing approximations of the dual solution.

We notice the presence of both the exact velocity u and a computed velocity U_h as coefficients in the dual problem. Below we will compute approximations of the dual solution where we replace u by U_h in the dual problem, an issue which we discuss below.

In [16] we prove the following error representation, where we express the total error as a sum of error contributions from the different elements K in space (assuming here for simplicity that the space mesh is constant in time), and we use the subindex K to denote integration over element K so that $(\cdot,\cdot)_K$ denotes the appropriate $L_2(K)$ inner product:

Theorem 1 *If (u,p) is the exact Navier-Stokes solution, (U_h,P_h) is a cG(1)cG(1) solution, (φ,θ) is the dual solution satisfying (9), and Φ and Θ are finite element functions satisfying $\Phi=\phi$ on Γ_0 and $\Phi=0$ on Γ_1, then*

$$|N(\sigma(u,p)) - N^h(\sigma(U_h,P_h))| = |\sum_{K\in\mathcal{T}_n}\mathcal{E}_K|,$$

where $\mathcal{E}_K = e_D^K + e_M^K$ with

$$\begin{aligned} e_D^K =& \frac{1}{|I|}\int_I \Big((\dot{U}_h + U_h\cdot\nabla U_h - f, \varphi-\Phi)_K - (P_h, \nabla\cdot(\varphi-\Phi))_K \\ &+ (\nabla\cdot U_h, \theta-\Theta)_K + (2\nu\epsilon(U_h), \epsilon(\varphi-\Phi))_K\Big)\, dt, \\ e_M^K =& \frac{1}{|I|}\int_I SD(\delta, U_h, P_h, \Phi, \Theta)_K\, dt. \end{aligned}$$

We may view e_D^K as the error contribution from the discretization on element K, and e_M^K as the contribution from the subgrid model on element K.

From the error representation in Theorem 1 there are various possibilities to construct error indicators and stopping criterions in an adaptive algorithm. Using standard interpolation estimates, with (Φ,Θ) a finite element interpolant of (φ,θ), we may estimate the contribution e_D^K from discretization as follows (cf. [8])

$$\begin{aligned} e_D^K \le \frac{1}{|I|}\int_I \Big(&(|R_1(U_h,P_h)|_K + |R_2(U_h,P_h)|_K)\cdot(C_h h^2|D^2\varphi|_K + C_k k|\dot{\varphi}|_K) \\ &+ \|R_4(U_h)\|_K (C_h h^2\|D^2\theta\|_K + C_k k\|\dot{\theta}\|_K)\Big)\, dt, \end{aligned}$$

where the residuals R_i are defined in (4), D^2 denotes second order spatial derivatives, and we write $|w|_K \equiv (\|w_1\|_K, \|w_2\|_K, \|w_3\|_K)$, with $\|w\|_K = (w,w)_K^{1/2}$, and let the dot denote the scalar product in $\mathbb{R}^3$.

The next step involves replacing the exact dual solution (φ,θ) by a computed approximation (φ_h,θ_h) obtained using cG(1)cG(1) on (usually) the same mesh as we use for the primal problem. Doing so we are led to the following a posteriori error estimate:

$$|N(\sigma(u,p)) - N^h(\sigma(U_h,P_h))| \approx |\sum_{K\in\mathcal{T}_n}\mathcal{E}_{K,h}| \tag{10}$$

where $\mathcal{E}_{K,h} = e^K_{D,h} + e^K_{M,h}$ with

$$e^K_{D,h} = \frac{1}{|I|}\int_I \Big((|R_1(U_h,P_h)|_K + |R_2(U_h,P_h)|_K) \cdot (C_h h^2 |D^2\varphi_h|_K + C_k k|\dot{\varphi}_h|_K) \\ + \|R_4(U_h)\|_K \cdot (C_h h^2 \|D^2\theta_h\|_K + C_k k \|\dot{\theta}_h\|_K) \Big)\, dt,$$
$$e^K_{M,h} = \frac{1}{|I|}\int_I SD(\delta, U_h, P_h, \varphi_h, \theta_h)_K\, dt,$$

where we have replaced the interpolant (Φ, Θ) by (φ_h, θ_h). Again we may view $e^K_{D,h}$ as the error contribution from the discretization on element K, and $e^K_{M,h}$ as the contribution from the subgrid model on element K.

Remark 2 *Non-Dirichlet boundary conditions, such as slip conditions at lateral boundaries and transparant outflow conditions, introduce additional boundary terms in the error representation in Theorem 1. Since the dual solution for this example is small at such non-Dirichlet boundaries, we neglect the corresponing boundary terms in the computations.*

Remark 3 *In the computations we use $C_k = 1/2$ and $C_h = 1/8$ as constant approximations of the interpolation constants in Theorem 1. These values are motivated by simple analysis on reference elements.*

5.3 An adaptive algorithm

In the computations we use Adaptive DNS/LES cG(1)cG(1) with an algorithm for adaptive mesh refinement in space (with for simplicity the space mesh and time steps constant in time) based on the a posteriori error estimate (10), of the form: Given an initial coarse computational space mesh $\mathcal{T}^0$, start at $k = 0$, then do

(1) Compute approximation to the primal problem using $\mathcal{T}^k$.
(2) Compute approximation to the dual problem using $\mathcal{T}^k$.
(3) If $|\sum_{K\in\mathcal{T}_k} \mathcal{E}^k_{K,h}| < TOL$ then STOP, else:
(4) Refine a fraction of the elements in $\mathcal{T}^k$ with largest $\mathcal{E}^k_{K,h} \rightarrow \mathcal{T}^{k+1}$.
(5) Set $k = k+1$, then goto (1).

6 Numerical example: surface mounted cube

We now study certain key features of Adaptive DNS/LES, in the form of the flow around a surface mounted cube at $Re = 40.000$, a benchmark problem at the *CDE-Forum* [1].

The cube side length is $H = 0.1$, and the cube is centrally mounted on the floor of a rectangular channel of length $15H$, height $2H$, and width $7H$, at a distance of $3.5H$ from the inlet. The cube is subject to a Newtonian flow (u, p) governed by the Navier-Stokes equations (1) with kinematic viscosity $\nu = 2.5 \cdot 10^{-6}$ and a unit inlet bulk velocity corresponding to a Reynolds number of 40.000, using the dimension of the cube as characteristic dimension. The inlet velocity profile is interpolated from experiments, and is avaliable for download at *CDE-Forum* [1], we use no slip boundary conditions on the cube and the vertical channel boundaries, slip boundary conditions on the lateral channel boundaries, and a transparent outflow boundary condition. This flow is very complex with a combination of laminar and turbulent features including boundary layers and a large turbulent wake, for further details see [12,13].

We seek to compute the *mean drag coefficient* $\bar{c}_D$ over a time interval $I = [0, 40H]$ at fully developed flow, defined by

$$\bar{c}_D = \frac{1}{|I|} \int_I c_D, \qquad \bar{c}_D \equiv \frac{2N(\sigma(u,p))}{\bar{U}_h^2 A}, \tag{11}$$

where $c_D(t)$ is the drag coefficient at time t, we set $\bar{U}_h = 1$ based on the bulk inflow velocity, the area $A = H \times H = H^2$, and $\phi = (1, 0, 0)$ in (6), the definition of $N(\sigma(u,p))$, with x_1 the direction of the channel. In the same way we define the *mean lift coefficient* $\bar{c}_L$ over the same time interval by (11), with now $\phi = (0, 1, 0)$ in (6) and x_2 the positive vertical direction of the channel.

We obtain approximations of $\bar{c}_D$ and $\bar{c}_L$ by using $N^h(\sigma(U_h, P_h))$ as an approximation of $N(\sigma(u,p))$. Using instead $N(\sigma(U_h, P_h))$ in the evaluation of $\bar{c}_D$ and $\bar{c}_L$, and thus neglecting the contribution from the stabilizing term (subgrid model), gives a slightly different result, in particular on very coarse meshes. On the finer meshes in the computations presented below, these differences are less significant, of the order 5% or less.

In Figure 1 we present results from [12] using the adaptive algorithm in Section 5.3 to compute $\bar{c}_D$ over a time interval of length $40H$. The approximations of $\bar{c}_D$ approaches ≈ 1.5, a value that is well captured already using less than 10^5 mesh points. We know of no experimental reference values of $\bar{c}_D$, but in [19] computational approximations are presented. The computational setup is similar to the one in [12] except the numerical method, a different length of the time interval, and that we in this paper use a channel of length $15H$ compared to a channel of length $10H$ in [19]. Using LES with different meshes and subgrid models, approximations of $\bar{c}_D$ in the interval $[1.14, 1.24]$ are presented in [19].

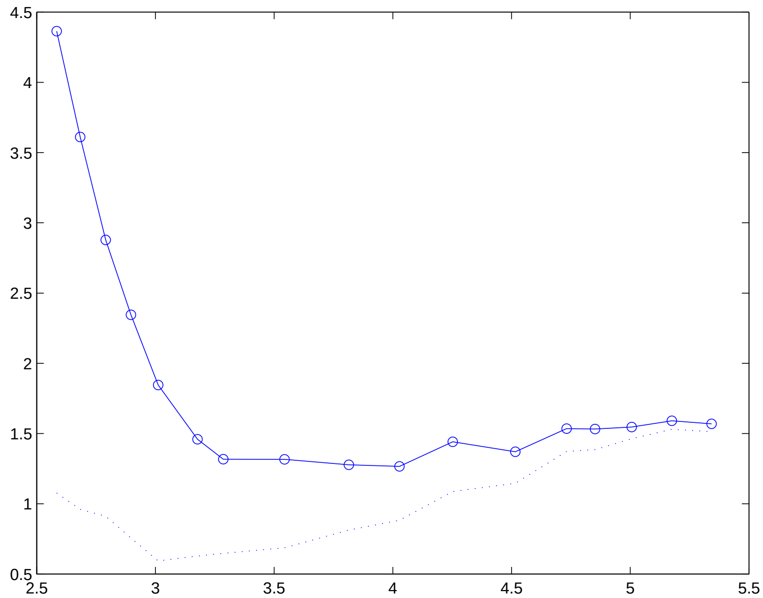

Figure 1. Approximations of the mean drag coefficient $\bar{c}_D$ ('o'), and the corresponding approximations without the contribution from the stabilizing term (':'), as functions of the 10-logarithm of the number of mesh points.

6.1 The dual solutions

A snapshot of a dual solution corresponding to the computation of the mean drag is shown in Figure 2, and in Figure 3 we plot a dual solution from [12], corresponding to the computation of the mean lift.

We note that both dual solutions are of moderate size, and in particular are not exploding as pessimistic worst case analytical estimates may suggest, but rather seems to behave as if the net effect of the crucial reaction term (with large oscillating coefficient ∇U_h) is only a moderate growth. The resulting computational meshes after 14 adaptive mesh refinements are shown in Figure 2 and Figure 3, respectively. We note that (φ_h, θ_h) is very concentrated in space, thus significantly influencing the adaptive mesh refinement. The initial space mesh is uniform and very coarse, 384 mesh points, and without the dual weights in the a posteriori error estimate the meshes would come out quite differently. We note the differences in the dual solutions for computation of drag as compared to lift.

6.2 A posteriori error estimates

In Figure 4 we plot the a posteriori error estimates $e_{D,h} + e_{M,h}$ from (10), as well as the true error based on the computational approximation on the finest mesh. The modeling error $e_{M,h}$ consists of sums in space and time of integrals over the space-time elements, and we may want to use a more conservative estimate of this term

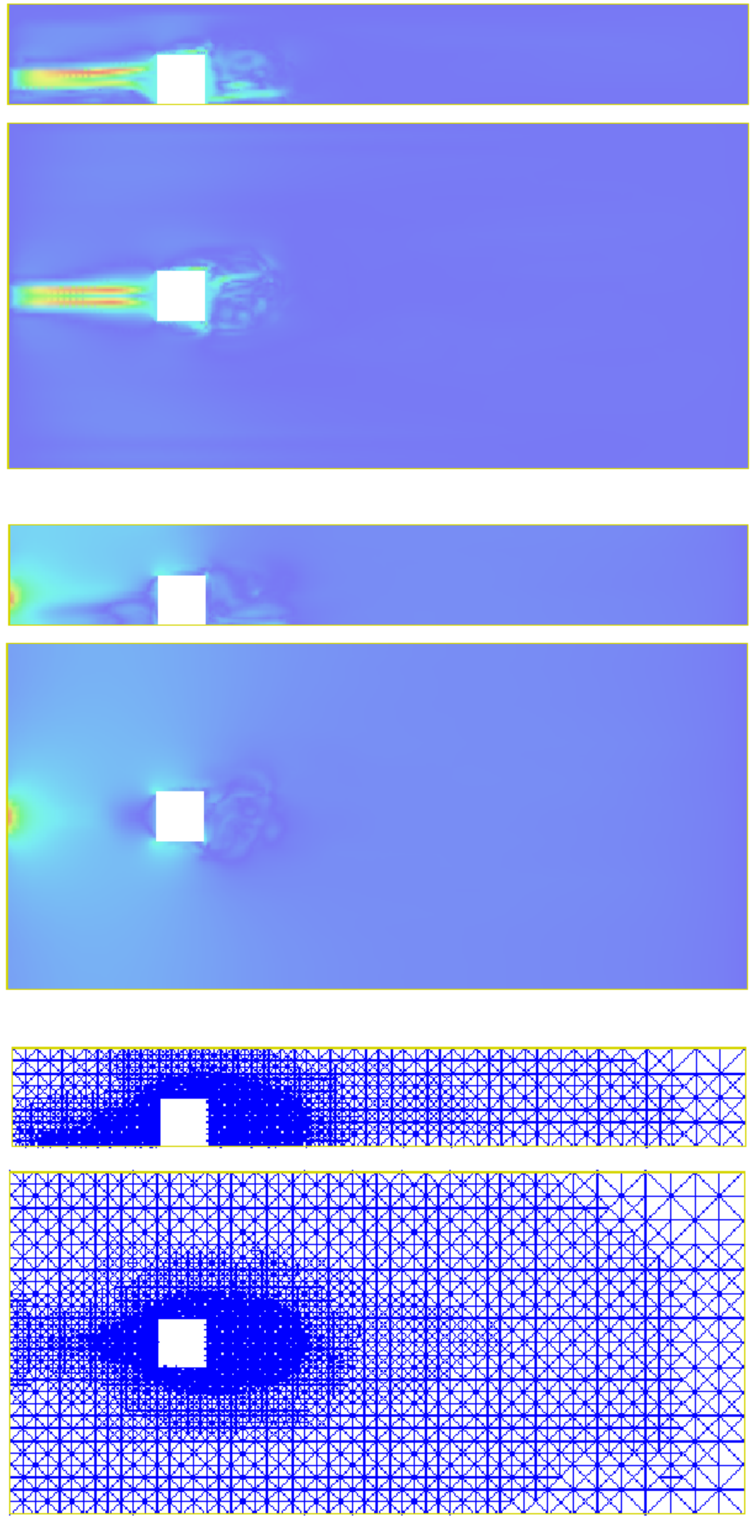

Figure 2. Dual velocity $|\varphi|$ (upper), dual pressure $|\theta|$ (middle), and the resulting computational mesh (lower), after 14 adaptive mesh refinements with respect to mean drag, in the x_1x_2-plane at $x_3 = 3.5H$ and in the x_1x_3-plane at $x_2 = 0.5H$.

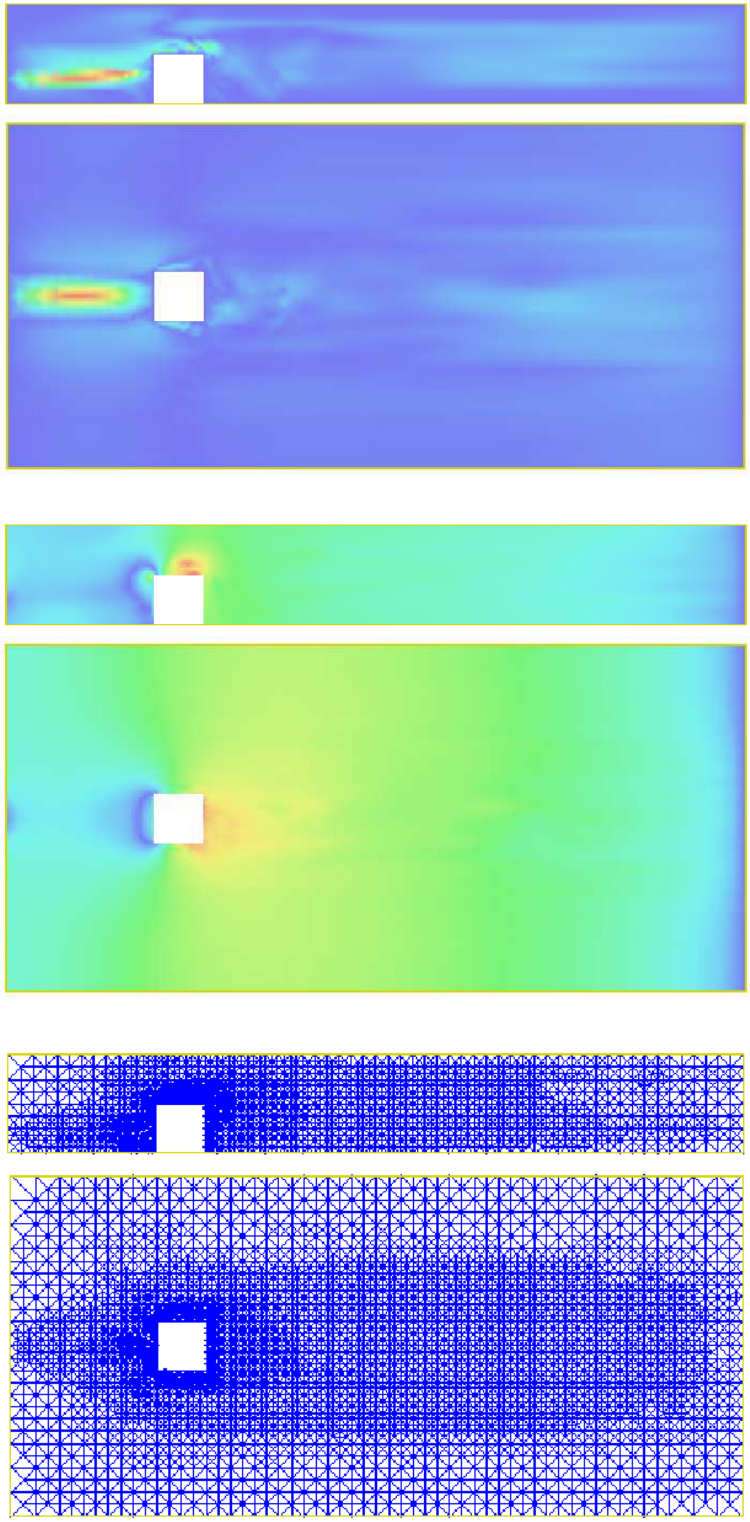

Figure 3. Dual velocity $|\varphi|$ (upper), dual pressure $|\theta|$ (middle), and the resulting computational mesh (lower), after 14 adaptive mesh refinements with respect to mean lift, in the x_1x_2-plane at $x_3 = 3.5H$ and in the x_1x_3-plane at $x_2 = 0.5H$.

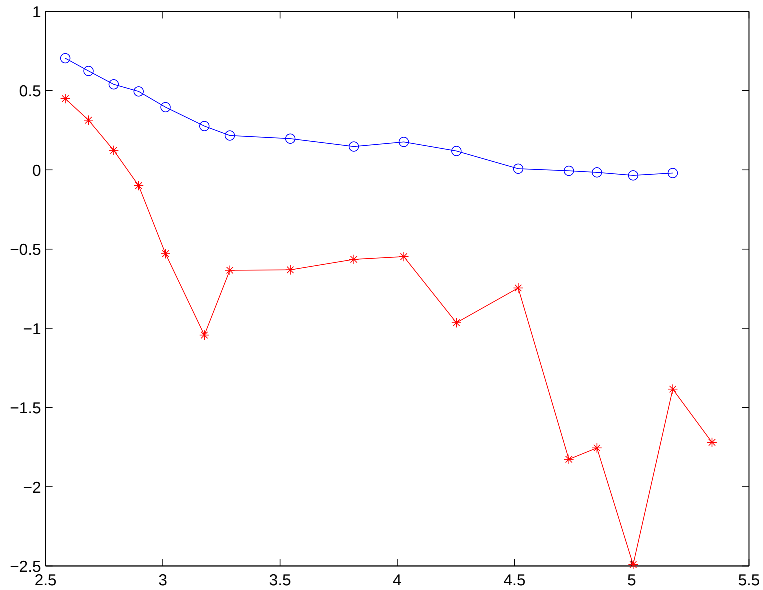

Figure 4. Log_{10}-$\log_{10}$ plot of the a posteriori error estimates $e_{D,h} + e_{M,h}$ ('o') for $\bar{c}_D$, vs the true error ('*') based on $\bar{c}_D = 1.55$, as functions of the number of mesh points in space.

by taking the absolute values inside any or both of these sums. In the evaluation of $e_{M,h}$ in Figure 4, we have set the absolute values inside the sums in space and time.

The a posteriori error estimates seem to over estimate the error with about a factor 4-5, and we find that once the value for $\bar{c}_D$ has stabilized, the a posteriori error estimates indicate that it may be hard to further increase the precision. This may be related to the fact that to further increase the precision, a better pointwise approximation of the trajectories of the true c_D is demanded, which may be very expensive. Such an increased precision may not even be desired, since the actual trajectories may be sensitive even for very small perturbations, and thus it is typically very hard to replicate also experiments with identical c_D trajectories. This couples to the question of *uniqueness in output*, a concept of uniqueness of weak solutions to the Navier-Stokes equations introduced in [17].

7 Reliability and efficiency of the adaptive method

We now forcus, in the context of the above computational example, on two key points relating to the *reliability* and *efficiency* of the adaptive method based on the a posteriori error estimate (10), which directly couples to whether this estimate indeed gives a reasonably sharp bound of the true error, or not. The two key points are (i) replacement of u by a computed velocity U_h in the dual problem, and (ii) replacement of the dual solution (φ, θ) by a computed dual solution (φ_h, θ_h). We may view both these points to relate to a *stability* of the dual solution under perturbations of (i) the convection coefficient and (ii) numerical computation. To test such stability we check the variation of certain key aspects of the dual solution computed on the different meshes, as measured in a couple of different norms as functions of the number of mesh points in space.

We first focus on the discretization error term $e_{D,h}$. We obtain a rough estimate of this term using Cauchy's inequality in space and time as follows (taking only space discretization coupled to φ into account and neglecting the small ν-term):

$$e_{D,h} \leq C_h \|hR_1(U_h, P_h)\| \|hD^2\varphi_h\|$$

where the interpolation constant $C_h \approx 1/8$, and by the least squares stabilization in cG(1)cG(1) we have that $\|\sqrt{h}R_1(U_h, P_h)\|$ is bounded (recalling that $\delta_1 \sim h$, and neglecting the time derivative). Here $\|\cdot\| = \|\cdot\|_{L_2(I;L_2(\Omega))}$ denotes a L_2 norm in space-time. Thus, very roughly we would expect to have

$$e_{D,h} \leq C_h \sqrt{h} \|hD^2\varphi_h\|.$$

The motivation for estimating the interpolation error in terms of higher order derivatives is to sharpen the a posteriori error estimates. Indeed, if we compare the three possible dual weights: $h^{-1}\varphi$, $1/2 \times \nabla\varphi$, and $1/8 \times hD^2\varphi$, with $1/2$ the interpolation constant corresponding to an interpolation estimate in terms of first order derivatives, we find in Figure 5 that the weight with the second order derivatives gives the sharpest estimate, and we find that after some initial refinements the dual solution shows a stability of this weight under the mesh refinement.

Next, the error contribution from subgrid modeling $e_{M,h} = SD(\delta, U_h, P_h, \varphi_h, \theta_h)$ may be estimated roughly as follows, using the basic energy estimate to bound $SD(\delta, U_h, P_h, U_h, P_h)$, Cauchys inequality, and recalling that $\delta_1 \sim h$, to get

$$e_{M,h} \leq \sqrt{h} \|\nabla\varphi_h\|$$

where we only accounted for the φ_h term. We notice in Figure 5 that $\|\nabla\varphi_h\|$ is of moderate size during the refinement, suggesting that indeed $e_{M,h}$ may get below a moderate tolerance under mesh refinement without reaching a DNS.

Altogether, we conclude that the crucial computed dual weights show a stability under mesh refinement which indicates that the a posteriori error estimate (10) for the discretization may indeed be reliable and also reasonably efficient.

Concerning the crucial step of replacing u by U_h in the dual problem, which may correspond to locally a large perturbation since U_h cannot be expected to pointwise approximate u, we have in particular given evidence that the net effect on the dual weights may be small.

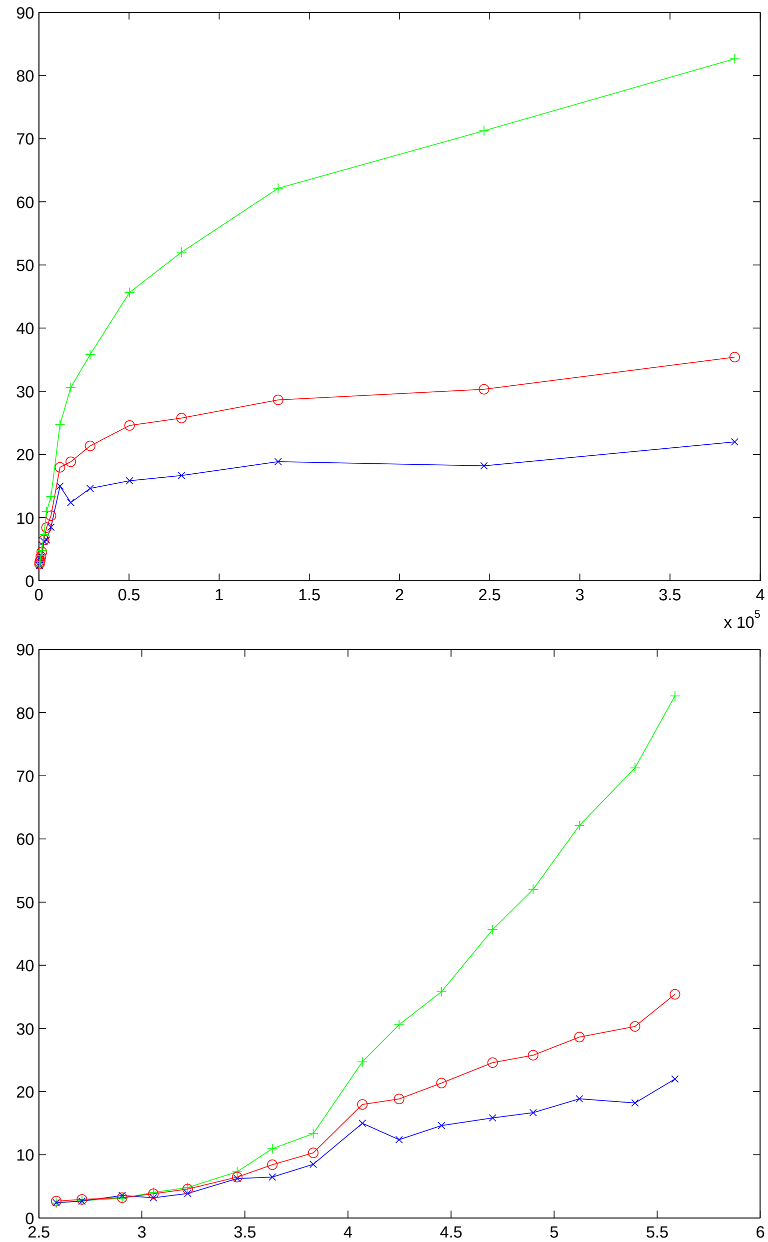

Figure 5. Stability factors $\|h^{-1}\varphi\|$, $1/2 \times \|\nabla\varphi\|$, and $1/8 \times \|h^1 D^2\varphi\|$, as functions of the number of mesh points in space (upper), and as functions of the 10-logarithm of the number of mesh points in space (lower).

8 Uniqueness in output of weak solutions to the Navier-Stokes equations

The stability of $\|\nabla\varphi\|$ is of particular interest, since the boundness of this quantity in fact implies *uniqueness in output* of a weak solution to the Navier-Stokes equations, which closely couples to the Clay $1 million Prize problem of the proof of existence and smoothiness of a solution to the Navier-Stokes equations, see [17].

Thus, in using Adaptive DNS/LES to compute a certain output from the Navier-Stokes equations, one is given, for free, computational evidence of uniqueness of that particular output, through the study of the stability of the corresponding dual solution. Not only is it possible this way to asses the output uniqueness of weak solutions, but we also obtain a quantitative measure of the computational cost associated with the computation of the given output.

Acknowledgments

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