THE DAS-MOSER COMMUTATOR CLOSURE FOR FILTERING THROUGH A BOUNDARY IS WELL POSED

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Abstract. When filtering through a wall with constant averaging radius, in addition to the subfilter scale stresses, a non-closed commutator term arises. We consider a proposal of Das and Moser to close the commutator error term by embedding it in an optimization probem. This report shows that this optimization based closure, with a small modification, leads to a well posed problem showing existence of a minimizer. We also derive the associated first order optimality conditions.

Key words. Turbulence, large eddy simulation, optimal control, Navier-Stokes, commutator error.

1. Introduction. Large eddy simulation is about approximating local spatial averages of fluid velocities in turbulent flows. Within this general idea there are very many possible choices and avenues of development. In one classical approach to LES local averages are defined by convolution with a selected filter kernel, such as (to fix ideas) a Gaussian,

$$\begin{aligned} \overline{u}(x,t) &:= g_\delta \star u(x,t), \text{ where} \\ g_\delta(x) &:= \delta^{-3} g(x/\delta), \text{ and } g(x) := Gaussian, \\ g_\delta \star u(x,t) &:= \int_{\mathbb{R}^3} g_\delta(x')u(x-x',t)dx'. \end{aligned}$$

For fixed averaging radius δ and in the absence of walls, filtering and differentiation commute and, in this simplified case, the Space Filtered NSE arise

$$\overline{u}_t + \nabla\cdot(\overline{u\otimes u}) + \nabla\cdot\sigma(\overline{u},\overline{p}) = \overline{f}(x) \text{ and } \nabla\cdot\overline{u} = 0,$$
$$\text{where } \sigma(u,p) := pI - 2\nu\nabla^s u, \text{ and } \nabla^s u := \frac{1}{2}[\nabla u + (\nabla u)^{tr}].$$

In the presence of walls, the picture becomes much more complex. One approach, is to decrease the averaging radius $\delta = \delta(x) \to 0$ as $x \to \partial\Omega$ as one approaches the wall so that no-slip boundary conditions can be imposed, see e.g. [26, 7]. This approach has independent importance, interest, development and challenges (such as loss of commutativity between differentiation and filtering and resolution of boundary layers that reappear in this formulation) but is not considered herein. Another approach, which we consider herein, is to keep a constant averaging radius, extend velocities by zero off the flow domain Ω and filter through the wall which we take to be the boundary of the flow domain $\Gamma := \partial\Omega$. If practicable, this has the great advantage of not requiring resolution of wall layers.

However, in the presence of walls (with the no-slip condition on $\partial\Omega$), filtering with constant averaging radius δ only commutes with some terms but not the divergence of the stress, a linear term. A careful derivation of the SFNSE in the presence of walls in [14], [13] (and independently by Das and Moser [9] around the same time) has shown

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that the correct equation, including the commutation error term that arises, is given by

$$\overline{u}_t + \nabla \cdot (\overline{u \otimes u}) - \nu \triangle \overline{u} + \nabla \overline{p} + A_\delta(u,p) = \overline{f}(x) \text{ and } \nabla \cdot \overline{u} = 0$$
$$\text{where } \; A_\delta(\sigma(u,p) \cdot \widehat{n}) = \int_\Gamma (\sigma(u,p) \cdot \widehat{n})(x') g_\delta(x - x') dx'$$
$$\text{and } \widehat{n} = \text{outward unit normal to } \Gamma.$$

The term A_δ decays rapidly as one moves away from the wall either into the domain or off the domain. The importance of the extra term which is not negligible is underlined by the following result of [14]. (For more recent studies of the detailed structure of A_δ see [2, 3, 19, 5, 6, 16]). This result shows that for fixed averaging radius the commutation error term must be modeled to attain any reasonable accuracy in LES, especially if the flow structures are created by turbulent flows interacting with walls.

THEOREM 1.1. *[14] The commutator error term*

$$\int_\Omega |A_\delta(\sigma(u,p) \cdot \widehat{n})|^2 dx \to 0 \;\; \textit{as } \delta \to 0$$

if and only if

$$\sigma(u,p) \cdot \widehat{n} \equiv 0 \quad \textit{on } \partial\Omega.$$

Das and Moser [4, 8, 9] proposed a closure for this critical commutator error term using optimization ideas and their intuition about the phenomenology related to the term. This paper considers this formulation from a mathematical viewpoint. We prove that the Das and Moser optimization closure, with a small adjustment, leads to a well posed problem and thus can be viewed as a general technique for arbitrary flows, geometries and other parameters. To explain the formulation of Das and Moser, a bit of extra geometry is needed.

DEFINITION 1.2. *Let the flow domain be denoted by $\Omega \subset \mathbb{R}^d, d = 2,3$, and suppose it is a bounded regular domain. Let Ω_δ denote the $O(\delta)$ width strip surrounding Ω and $\widetilde{\Omega}$ the extended domain:*

$$\Gamma = \partial\Omega,$$
$$\Omega_\delta := \{x \notin \Omega : dist(x, \Gamma) < \delta\},$$
$$\widetilde{\Omega} := interior(\overline{\Omega_\delta \cup \Omega}),$$

First note that if $g_\delta(x) = 0$ for $|x| \geq \delta$ then by this construction the true flow averages $\overline{u}$ vanish on the boundary of the extended domain. For the Gaussian filter, the exponential decay of the gaussian implies that the true flow averages will be exponentially close to zero there as well. Thus, boundary conditions for the flow averages on the boundary of the extended domain are clear:

$$\overline{u} = 0 \text{ on } \partial\widetilde{\Omega}.$$

The next closure issue is the commutator error term. Das and Moser [9] proposed the following. Let v denote a proxy variable for the unknown normal stress $\sigma \cdot n$ on Γ. The unknown function v is chosen to minimize the momentum transport through Γ into the extension strip Ω_δ:

$$J(\overline{u}, v) := \frac{1}{T} \int_0^T \int_{\Omega_\delta} \frac{1}{2} |\overline{u}(x,t)|^2 + \frac{\alpha}{2} |\overline{u}_t(x,t)|^2 dx dt. \tag{1.1}$$

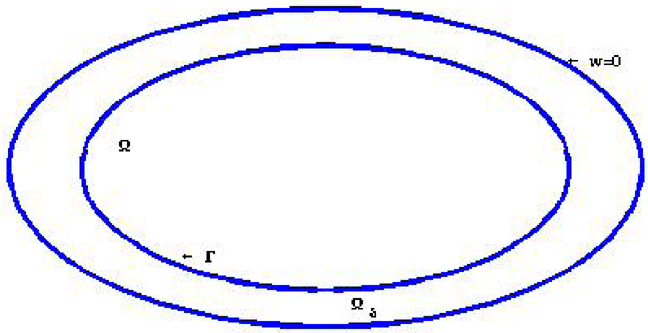

Fig. 1.1: Computational domain

The constant α has units $[\alpha] = \text{time}^2$. For (extensive) computational tests of this commutator closure (1.1) see [8, 9, 10, 24]. The goal of this report is to complement those works on the phenomenology and the accuracy of (1.1) by proving its universal solvability and well posedness.

Remark 1.1. *Aside from the Das Moser commutator closure (studied herein), there are other studies using optimization ideas in LES. For example, if benchmark flow data is known for the particular setting, parameters in near wall models (e.g. [20, 25]) can be used to control the flow to the benchmark values, as studied by [27, 28, 29, 30].*

1.1. Formulation of the main result. To present our result a bit more development is needed. First, closure of the subfilter scale stresses must be addressed. It is well known , e.g., [26, 19], that

$$R(u,u) := \overline{u \otimes u} - \overline{u} \otimes \overline{u}$$

is not closed and must be replaced by a term that depends only on the flow averages. There are very many such models and the exact choice is not central to this work herein. We represent it as

$$R(u,u) \Leftarrow S(\overline{u},\overline{u}).$$

When this substitution is made for closure the model solution is no longer the flow averages but a (hopefully accurate) approximation of them, see e.g. [19, 26]. Thus we denote:

$$w(x,t) := \text{ LES approximation of the true flow averages } \overline{u}(x,t).$$

To ensure universal solvability, the target functional (1.1) must be augmented by terms to ensure that the controller does not require infinite energy. Thus, we so augment the functional (1.1) to obtain

$$J_\beta(w,v) := \frac{1}{T}\int_0^T\!\!\int_{\Omega_\delta} \frac{1}{2}|w(x,t)|^2 + \frac{\alpha}{2}|w_t(x,t)|^2 \, dxdt \qquad (1.2)$$
$$+ \frac{\beta}{2}\frac{1}{T}\int_0^T\!\!\int_\Gamma |v(x',t)|^2 dx'dt + \frac{\gamma}{2}\int_{\Omega_\delta} |w(x,T)|^2 dx.$$

We therefore consider the problem:

$$
\begin{aligned}
&\text{minimize}_v \quad J_\beta(w,v)\\
&\text{subject to :}\\
&w_t+\nabla\cdot(w\otimes w)-\nu\triangle w+\nabla q+\nabla\cdot S(w,w)-\int_\Gamma v(x',t)g_\delta(x-x')dx' \qquad (1.3)\\
&\qquad=\overline{f}(x,t)\ ,\ x\in\widetilde{\Omega},0<t\le T,\\
&\nabla\cdot w=0,\ x\in\widetilde{\Omega},0<t\le T,\\
&w=0,\ \text{on}\ \partial\widetilde{\Omega},0<t\le T,\\
&w(x,0)=\overline{u}(x,0),x\in\widetilde{\Omega}.
\end{aligned}
$$

The subfilter scale model is secondary herein to the closure model. To simplify our presentation we take the Smagorinsky model, see e.g. [28, 21], (which is not the state of the art)

$$S(w,w)=-\varepsilon|\nabla w|^{r-2}\nabla w$$

for which exists a globally unique strong solution for $r\ge\frac{11}{5}$ [23, 22].

2. Existence of a minimizer.

We begin by proving that the Das Moser closure is well-posed.

THEOREM 2.1. *Let $\overline{u}_0\in H_0^1(\widetilde{\Omega})\cap W^{1,r}(\widetilde{\Omega})$, $r\ge\frac{11}{5}$. There exists an optimal pair (w^*,v^*) solution for the minimization problem (1.3), where $w^*\in H^1([0,T];L^2(\widetilde{\Omega}))\cap L^\infty(0,T;W^{1,r}(\widetilde{\Omega}))\cap L^2(0,T;H^2(\widetilde{\Omega}))\cap L^r(0,T,W^{1,3r}(\widetilde{\Omega}))$, and $v^*\in L^2(0,T;L^2(\Gamma))$.*

Proof. The argument is standard, see e.g. [1, 17, 15, 12], but we sketch it for reader's convenience. Let $\inf_{v,w}J_\beta(w,v)=d\in[0,\infty)$ and (w^n,v^n) a minimizing sequence:

$$
\begin{aligned}
d\le\int_0^T\!\!\int_{\Omega_\delta}\left(\frac12|w^n|^2+\frac{\alpha}{2}|w_t^n)|^2\right)dxdt+\frac{\beta}{2}\int_0^T\!\!\int_\Gamma|v^n|^2dx'dt&\\
+\frac{\gamma}{2}\int_{\Omega_\delta}|w^n(T)|^2dx<d+\frac1n.&
\end{aligned}
\qquad (2.1)
$$

From the above we have that $\{v^n\}_n$ is bounded in $L^2(0,T,L^2(\Gamma))$. Multiplying (1.3) by w^n and integrating by parts we obtain the following energy estimate (here $\|\cdot\|$ denotes the $\|\cdot\|_{L^2(\widetilde{\Omega})}$ norm, generated by the $\langle\cdot,\cdot\rangle_{L^2(\widetilde{\Omega})}$ inner product)

$$
\begin{aligned}
&\frac12\frac{d}{dt}\|w^n\|^2+\nu\|\nabla w^n\|^2+\varepsilon\|\nabla w^n\|^r_{L^r(\widetilde{\Omega})}=\langle\overline{f},w^n\rangle+\int_{\widetilde{\Omega}}w^n\left(\int_\Gamma v^n(x',t)g(x-x')dx'\right)dx\\
&\le\frac12\|f\|^2+\frac12\|w^n\|^2\left(1+C(\widetilde{\Omega},\Gamma,\delta)\|v^n(\cdot,t)\|^2_{L^2(\Gamma)}\right)
\end{aligned}
$$

and by (2.1) and Grönwall inequality

$$\|w^n(t)\|^2+\int_0^T\left(\nu\|\nabla w^n(t)\|^2+\varepsilon\|\nabla w^n\|_r^r\right)dt\le C(\widetilde{\Omega},\Gamma,\delta) \qquad (2.2)$$

for all $t\in[0,T]$. Here and in the sequel we denote by $C=C(\widetilde{\Omega},\Gamma,\delta)$ several constants that depend only on $T,\widetilde{\Omega},\Gamma,\delta$ and ν.

Multiplying (1.3) by $-\Delta w^n$ and integrate by parts, after some calculations using (see e.g. [11])

$$\|\nabla w^n\|_{3r}^r \leq \langle \nabla \cdot |\nabla w^n|^{r-2} \nabla w^n, \Delta w^n \rangle$$

we obtain

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\|\nabla w^n\|^2 + \nu\|\Delta w_n\|^2 + \varepsilon\|\nabla w\|_{3r}^r \\
&= \langle w^n \cdot \nabla w^n, \Delta w^n \rangle - \langle \overline{f}, \Delta w^n \rangle - \int_{\widetilde{\Omega}} \Delta w^n \left(\int_\Gamma v^n(x',t) g(x-x') dx' \right) dx \\
&\leq \|\nabla w^n\|_3^3 + \frac{\nu}{2}\|\Delta w^n\|^2 + \frac{1}{\nu}\|\overline{f}\|^2 + \frac{C(\widetilde{\Omega},\Gamma,\delta)}{\nu}\|v^n\|_{L^2(\Gamma)}^2
\end{aligned}$$

and for $3 \leq r$

$$\frac{d}{dt}\|\nabla w^n\|^2 + \nu\|\Delta w_n\|^2 + 2\|\nabla w\|_{3r}^r \leq C(\widetilde{\Omega},\Gamma,\delta)\left(1 + \|\overline{f}\|^2 + \|v^n\|_{L^2(\Gamma)}^2\right)$$

while for $\frac{11}{5} \leq r < 3$, $\lambda = \frac{2(3-r)}{3r-5}$ (see [11])

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\|\nabla w^n\|^2 + \nu\|\Delta w_n\|^2 + \|\nabla w\|_{3r}^r \\
&\leq C\|\nabla w^n\|_2^{2\lambda}\|\nabla w^n\|_r^r + \frac{\nu}{2}\|\Delta w^n\|^2 + \frac{1}{\nu}\|\overline{f}\|^2 + \frac{C(\widetilde{\Omega},\Gamma,\delta)}{\nu}\|v^n\|_{L^2(\Gamma)}^2
\end{aligned}$$

i.e.,

$$\begin{aligned}
&\frac{d}{dt}\|\nabla w^n\|^2 + \nu\|\Delta w_n\|^2 + 2\|\nabla w\|_{3r}^r \\
&\leq C\|\nabla w^n\|_2^{2\lambda}\|\nabla w^n\|_r^r + \frac{2}{\nu}\|\overline{f}\|^2 + \frac{C(\widetilde{\Omega},\Gamma,\delta)}{\nu}\|v^n\|_{L^2(\Gamma)}^2
\end{aligned}$$

and by (2.2)

$$\|\nabla w^n(t)\|^2 + \int_0^T \left(\nu\|\Delta w^n(t)\|^2 + \|\nabla w^n\|_{3r}^r\right) dt \leq C, \tag{2.3}$$

for all $t \in [0,T]$. This implies the uniform bound of w^n in $L^\infty(0,T;H_0^1(\widetilde{\Omega})) \cap L^2(0,T;H^2(\widetilde{\Omega})) \cap L^r(0,T;W^{1,3r}(\widetilde{\Omega}))$.
Multiplying (1.3) by w_t^n and integrating by parts we obtain

$$\begin{aligned}
&\|w_t^n\|^2 + \frac{\nu}{2}\frac{d}{dt}\|\nabla w_n\|^2 + \frac{\varepsilon}{r}\frac{d}{dt}\|\nabla w\|_r^r \\
&= -\langle w^n \cdot \nabla w^n, w_t^n \rangle + \langle \overline{f}, w_t^n \rangle + \int_{\widetilde{\Omega}} w_t^n \left(\int_\Gamma v^n(x',t) g(x-x') dx' \right) dx \\
&\leq \|w_t^n\| \left(\|w^n \cdot \nabla w^n\| + \|f\| + C\|v^n\|_{L^2(\Gamma)}\right) \\
&\leq \frac{1}{2}\|w_t^n\|^2 + \frac{1}{2}2\left(\|w^n \cdot \nabla w^n\|^2 + \|f\|^2 + C^2\|v^n\|_{L^2(\Gamma)}^2\right) \\
&\leq \frac{1}{2}\|w_t^n\|^2 + \left(\|w^n\|_{\frac{6r}{3r-2}}^2\|\nabla w^n\|_{3r}^2 + \|f\|^2 + C^2\|v^n\|_{L^2(\Gamma)}^2\right) \\
&\leq \frac{1}{2}\|w_t^n\|^2 + \left(C\|\nabla w^n\|^2\|\nabla w^n\|_{3r}^2 + \|f\|^2 + C^2\|v^n\|_{L^2(\Gamma)}^2\right)
\end{aligned}$$

equivalently

$$
\begin{aligned}
&\nu \frac{d}{dt}\|\nabla w^n\|^2 + \frac{2\varepsilon}{r}\frac{d}{dt}\|\nabla w^n\|_p^p + \|w_t^n\|^2 \le C\left(\|\nabla w^n\|^2\|\nabla w^n\|_{3r}^2 + \|f\|^2 + \|v^n\|_{L^2(\Gamma)}^2\right),\\
&\nu\|\nabla w^n(t)\|^2 + \frac{2\varepsilon}{r}\|\nabla w^n(t)\|_r^r + \int_0^T \|w_t^n(t)\|^2 dt\\
&\quad \le \nu\|\nabla w^n(0)\|^2 + \frac{2\varepsilon}{r}\|\nabla w^n(0)\|_r^r + C\int_0^T\!\left(\|\nabla w^n\|^2\|\nabla w^n\|_{3r}^2 + \|f\|^2 + \|v^n\|_{L^2(\Gamma)}^2\right) dt
\end{aligned}
$$

and by the Grönwall inequality and (2.2)-(2.3)

$$
\nu\|\nabla w^n(t)\|^2 + \varepsilon\|\nabla w^n(t)\|_r^r + \int_0^T \|w_t^n(t)\|^2 dt \le C. \tag{2.4}
$$

We conclude that for $w^n(0) \in W_0^{1,r}(\widetilde{\Omega})$, the sequence w^n is uniformly bounded in $L^\infty(0,T;W^{1,r}(\widetilde{\Omega})) \cap H^1(0,T;L^2(\widetilde{\Omega}))$.
From (2.2)-(2.4) and the weak lower-semicontinuity of the functional $J_\beta(w,v)$ we have

$$
\begin{aligned}
&\liminf_{n\to\infty} J_\beta(w^n,v^n)\\
&\quad \ge \int_0^T\!\!\int_{\Omega_\delta}\left(\frac{1}{2}|w^*|^2 + \frac{\alpha}{2}|w_t^*|^2\right) dxdt + \frac{\beta}{2}\int_0^T\!\!\int_\Gamma |v^*|^2 dx' dt + \frac{\gamma}{2}\int_{\Omega_\delta} |w^*(T)|^2 dx
\end{aligned}
$$

where, on a subsequence,

$$
\begin{array}{ll}
w^n \to w^* & \text{strongly in } C([0,T];L^2(\widetilde{\Omega})) \cap L^2(0,T;H_0^1(\widetilde{\Omega}))\\
w_t^n \rightharpoonup w_t^* & \text{weakly in } L^2(0,T;L^2(\widetilde{\Omega}))\\
\Delta w^n \rightharpoonup \Delta w^* & \text{weakly in } L^2(0,T;L^2(\widetilde{\Omega}))\\
v^n \rightharpoonup v^* & \text{weakly in } L^2(0,T;L^2(\Gamma)).
\end{array} \tag{2.5}
$$

On the other hand, due to the monotonicity of the Smagorinski nonlinear viscous term,

$$
0 \le \varepsilon \int_{\widetilde{\Omega}} \left(|\nabla w^n|^{r-2}\nabla w^n - |\nabla w^*|^{r-2}\nabla w^*\right)(\nabla w^n - \nabla w^*)\, dx
$$

and since

$$
\begin{aligned}
&\langle w^n\cdot\nabla w^n - w^*\cdot\nabla w^*, \varphi\rangle = \langle (w^n - w^*)\cdot\nabla w^*, \varphi\rangle + \langle w^n\cdot\nabla(w^n - w^*), \varphi\rangle\\
&\quad \le \|\nabla(w^n - w^*)\|\|\nabla w^*\|^{\frac{1}{2}}\|\Delta w^*\|^{\frac{1}{2}}\|\varphi\|\\
&\qquad + \|\nabla w^n\|\|\nabla(w^n - w^*)\|^{\frac{1}{2}}\|\Delta(w^n - w^*)\|^{\frac{1}{2}}\|\varphi\|
\end{aligned}
$$

we obtain from (2.5) that (w^*,v^*) satisfies (1.3), hence $J_\beta(w^*,v^*) = d$ and (w^*,v^*) is a minimizer. □

3. First-order necessary conditions of optimality. We now show that the optimal solution (w^*,v^*) must satisfy the first-order necessary condition associated with the optimal control problem (1.3). By studying the case in which the Gâteaux derivative of the cost functional $J_\beta(w,v)$ vanishes, we get a possible candidate solution for the optimal state w^* and optimal control v^*, see e.g. [31].

3.1. Gâteaux differentiability. We now prove the existence of the Gâteaux derivative.

Lemma 3.1. *Let* $\overline{u}(\cdot,0) \in H_0^1(\widetilde{\Omega}) \cap W^{1,r}(\widetilde{\Omega})$. *The mapping* $w = w(v)$ *from* $L^2(0,T;L^2(\Gamma))$ *to* $L^2(0,T;H_0^1(\widetilde{\Omega}))$, *defined as the solution of (1.3), has a Gâteaux derivative* $(Dw/Dv)\cdot V$ *in every direction* V *in* $L^2(0,T;L^2(\Gamma))$. *Furthermore,* $W(V) = (Dw/Dv)\cdot V$ *is the solution of the problem*

$$\begin{aligned}
&W_t + w\cdot\nabla W + W\cdot\nabla w - \nu\Delta W - \varepsilon(p-1)\nabla\cdot(|\nabla w|^{r-2}\nabla W) + \nabla\widetilde{p} \\
&\qquad = \int_\Gamma V(x',\cdot)g(x-x')dx' \qquad \text{in } \widetilde{\Omega}\times(0,T), \\
&\nabla\cdot W = 0 \qquad \text{in } \widetilde{\Omega}\times(0,T), \\
&W = 0 \qquad \text{on } \partial\widetilde{\Omega}\times(0,T), \\
&W(\cdot,0) = 0 \qquad \text{in } \widetilde{\Omega}.
\end{aligned} \tag{3.1}$$

Proof. See, e.g., [18]. □

3.2. Necessary Conditions. The Gâteaux derivative gives information about the sensitivity of the system at a particular point w in a particular direction V, but complete information requires one to solve (3.1) for every possible direction V. In order to minimize the functional $J_\beta(w,v)$ we need only an integral over all these directions, which is obtained through the solution of an adjoint equation.

Theorem 3.2. *Let* (w^*,v^*) *be an optimal pair. Then*

$$v^*(x',t) = -\frac{1}{\beta}\int_{\widetilde{\Omega}} \lambda(x,t)g(x-x')dx, \qquad a.e.\ t\in(0,T),\ x'\in\Gamma, \tag{3.2}$$

where $\lambda \in W^{1,2}([0,T],L^2(\widetilde{\Omega}))\cap L^2(0,T;H_0^1(\widetilde{\Omega})\cap H^2(\widetilde{\Omega}))$, *satisfies the adjoint equation*

$$\begin{aligned}
&-\lambda_t - w^*\cdot\nabla\lambda + (\nabla w^*)^T\lambda - \nu\Delta\lambda - \varepsilon(r-1)\nabla\cdot\left(|\nabla w|^{r-2}\nabla\lambda\right) \\
&\qquad +\nabla\hat{p} = m(x)\,(w^* - \alpha w^*_{tt}) \quad \text{in } \widetilde{\Omega}\times(0,T), \\
&\nabla\cdot\lambda = 0 \qquad \text{in } \widetilde{\Omega}\times(0,T), \\
&\lambda = 0 \qquad \text{on } \partial\widetilde{\Omega}\times(0,T), \\
&\lambda(\cdot,T) = m(\cdot)(\alpha w^*_t(\cdot,T) + \gamma w^*(\cdot,T)) \qquad \text{in } \widetilde{\Omega}.
\end{aligned} \tag{3.3}$$

where $m(x)$ *is the characteristic function of the set* Ω_δ.

Proof. Let (w^*,v^*) be an optimal pair for the control problem (1.3) and take W to be the solution of the sensitivity equation (3.1) with $(w,v) := (w^*,v^*)$, for an arbitrary $V\in L^2(0,T;L^2(\Gamma))$. Then the optimality of (w^*,v^*) writes

$$0 \le \frac{dJ_\beta(v^*)}{dv}V, \qquad \text{for all } V\in L^2(0,T;L^2(\Gamma))$$

which by (1.2) and integration by parts it implies

$$
\begin{aligned}
0 &\leq \int_0^T\!\!\int_{\Omega_\delta} (w^* W + \alpha w_t^* W_t)\, dx dt + \beta \int_0^T\!\!\int_\Gamma v^* V\, dx' dt + \gamma \int_{\Omega_\delta} w^*(T) W(T) dx \\
&= \int_0^T\!\!\int_{\widetilde{\Omega}} m(x) \left(w^* W - \alpha w_{tt}^* W\right) dx dt + \alpha \int_{\Omega_\delta} w_t^* W \Big|_0^T dx \\
&\quad + \beta \int_0^T\!\!\int_\Gamma v^* V\, dx' dt + \gamma \int_{\Omega_\delta} w^*(T) W(T) dx.
\end{aligned}
$$

Now using the right hand-side of the adjoint equation (3.3) we have

$$
\begin{aligned}
0 \leq& \int_0^T\!\!\int_{\widetilde{\Omega}} W \left(-\lambda_t - w^* \cdot \nabla \lambda + (\nabla w^*)^T \lambda - \nu \Delta \lambda - \varepsilon (r-1) \nabla \cdot \left(|\nabla w|^{r-2} \nabla \lambda\right) + \nabla \hat{p}\right) dx dt \\
&+ \alpha \int_{\Omega_\delta} w_t^* W \Big|_0^T dx + \beta \int_0^T\!\!\int_\Gamma v^* V\, dx' dt + \gamma \int_{\Omega_\delta} w^*(T) W(T) dx \\
=& - \int_{\widetilde{\Omega}} W \lambda \Big|_0^T dx - \int_0^T\!\!\int_{\partial \widetilde{\Omega}} W \lambda w \cdot n d\sigma + \nu \int_0^T\!\!\int_{\partial \widetilde{\Omega}} (-W \nabla \lambda + \nabla W \lambda) \cdot n d\sigma \\
&+ \varepsilon (r-1) \int_0^T\!\!\int_{\partial \widetilde{\Omega}} \left(-W |\nabla w|^{r-2} \nabla \lambda + |\nabla w|^{r-2} \lambda \nabla W\right) \cdot n d\sigma \\
&+ \int_0^T\!\!\int_{\widetilde{\Omega}} \lambda \left(W_t + w^* \cdot \nabla W + W \cdot \nabla w^* - \nu \Delta W - \varepsilon (r-1) \nabla \cdot \left(|\nabla w|^{r-2} \nabla W\right) + \nabla \hat{p}\right) dx dt \\
&+ \alpha \int_{\Omega_\delta} w_t^* W \Big|_0^T dx + \beta \int_0^T\!\!\int_\Gamma v^* V\, dx' dt + \gamma \int_{\Omega_\delta} w^*(T) W(T) dx
\end{aligned}
$$

which by the sensitivity equation (3.1) yields

$$
\begin{aligned}
0 \leq& - \int_{\widetilde{\Omega}} W(x,\cdot) \lambda(x,\cdot) \Big|_0^T dx - \int_0^T\!\!\int_{\partial \widetilde{\Omega}} W \lambda w \cdot n d\sigma + \nu \int_0^T\!\!\int_{\partial \widetilde{\Omega}} (-W \nabla \lambda + \nabla W \lambda) \cdot n d\sigma \\
&+ \varepsilon (r-1) \int_0^T\!\!\int_{\partial \widetilde{\Omega}} \left(-W |\nabla w|^{r-2} \nabla \lambda + |\nabla w|^{r-2} \lambda \nabla W\right) \cdot n d\sigma \\
&+ \int_0^T\!\!\int_{\Omega_\delta} \lambda(x,t) \left(\int_\Gamma V(x',t) g(x-x') dx'\right) dx dt \\
&+ \alpha \int_{\Omega_\delta} w_t^*(x,\cdot) W(x,\cdot) \Big|_0^T dx + \beta \int_0^T\!\!\int_\Gamma v^* V\, dx' dt + \gamma \int_{\Omega_\delta} w^*(T) W(T) dx
\end{aligned}
$$

$$
\begin{aligned}
\leq& \int_{\widetilde{\Omega}} W(x,T) \left(-\lambda(x,T) + m(x) (\gamma w^*(x,T) + \alpha w_t^*(x,T))\right) dx \\
&+ \int_0^T\!\!\int_{\partial \widetilde{\Omega}} \left(-W \lambda w + \nu \left(-W \nabla \lambda + \nabla W \lambda\right) + \varepsilon (r-1) |\nabla w|^{r-2} (-W \nabla \lambda + \lambda \nabla W)\right) \cdot n d\sigma \\
&+ \int_0^T\!\!\int_\Gamma V(x',t) \left(\beta v^*(x',t) + \int_{\Omega_\delta} \lambda(x,t) g(x-x') dx\right) dx' dt
\end{aligned}
$$

Finally, we use again the adjoint equation (3.3) to obtain the first order necessary condition of optimality

$$0 \leq \int_0^T\!\!\int_\Gamma V(x',t)\left(\beta v^*(x',t) + \int_{\Omega_\delta} \lambda(x,t) g(x-x')dx\right) dx'dt = \frac{dJ_\beta(v^*)}{dv} V, \tag{3.4}$$

for all $V \in L^2(0,T;L^2(\Gamma))$, from which (3.2) is deduced. □

REMARK 3.1. *The final condition in (3.3) has $w_t(\cdot,T)$, while $w \in C([0,T], L^2(\widetilde{\Omega}))$, $w_t \in L^2(0,T;L^2(\widetilde{\Omega}))$. For conditions on the smoothness of w with respect to t, see e.g. [21].*

3.3. The optimality system. In order to obtain the solution of our control problem we have to solve for $w \in L^2(0,T;H_0^1(\widetilde{\Omega}))$, $q \in L^2(0,T;L_0^2(\widetilde{\Omega}))$, $\lambda \in L^2(0,T;H_0^1(\widetilde{\Omega}))$ and $\hat{p} \in L^2(0,T;L_0^2(\widetilde{\Omega}))$ the optimality system

$$\begin{cases} w' - \nu\Delta w + (w\cdot\nabla)w - \varepsilon\nabla\cdot\left(|\nabla w|^{r-2}\nabla w\right) + \nabla q & \\ \qquad = \overline{f} + \displaystyle\int_\Gamma v(x',t)g(x-x')dx' & \text{in } \widetilde{\Omega}\times(0,T), \\ \nabla\cdot w = 0 & \text{in } \widetilde{\Omega}\times(0,T), \\ w(\cdot,0) = w_0(\cdot) & \text{in } \widetilde{\Omega}, \\ -\lambda_t - w\cdot\nabla\lambda + (\nabla w)^T\lambda - \nu\Delta\lambda - \varepsilon(r-1)|\nabla w|^{r-2}\nabla\lambda + \nabla\hat{p} & \\ \qquad = m(x)(w - \alpha w_{tt}) & \text{in } \widetilde{\Omega}\times(0,T), \\ \nabla\cdot\lambda = 0 & \text{in } \widetilde{\Omega}\times(0,T), \\ \lambda(\cdot,T) = m(\cdot)(w_t(\cdot,T) + \gamma w(\cdot,T)) & \text{in } \widetilde{\Omega}, \\ \beta v(x',t) + \displaystyle\int_{\Omega_\delta}\lambda(x,t)g(x-x')dx = 0 & \text{on } \Gamma\times(0,T). \end{cases} \tag{3.5}$$

with homogeneous Dirichlet boundary conditions $w = \lambda = 0$ on $\partial\widetilde{\Omega}\times(0,T)$.

We note that $v \in C([0,T];C^\infty(\Gamma))$ and $w \in C([0,T];H_0^1(\widetilde{\Omega})) \cap L^2(0,T;H^2(\widetilde{\Omega}))$ for all finite values of α, β and γ.

3.4. A gradient algorithm. Due to the fact that the equation (1.3) marches forward in time from an initial condition and the adjoint equation (3.3) marches backward in time from a terminal condition, any practical algorithm would involve a split of the optimality system (3.5) into two parts.

We note that one method of splitting this system is by a gradient algorithm for the solution of the optimal control problem. Let κ be the iteration counter of the algorithm, $v(k)$ the κth iterate for the control and $J_\beta(\kappa) = J_\beta(w(\kappa), v(\kappa))$. At each iteration κ, the algorithm requires sequential solution of the state equation (1.3) and adjoint equation (3.3), following the gradient descent direction $\frac{dJ_\beta(v(\kappa))}{dv}$ given by (3.4).

The Gradient Algorithm

(a) initialization:
- (a1) choose tolerance τ and $v(0)$; set $\kappa = 0$ and gradient step size $\mu = 1$;
- (a2) compute $w(0)$ by solving (1.3) with $v = v(0)$
- (a3) evaluate $J_\beta(0)$;

(b) main loop:
- (b1) set $\kappa = \kappa + 1$;
- (b2) compute $\lambda(\kappa)$ from (3.3) with $w = w(\kappa - 1)$;

(b3) set $v(\kappa) = v(\kappa-1) - \mu\left(\beta v(\kappa-1) + \int_{\Omega_\delta} \lambda(\kappa) g\right)$
(b4) compute $w(\kappa)$ from (1.3) with $v = v(\kappa)$;
(b5) evaluate $\mathcal{J}_\beta(\kappa)$;
(b6) if $\mathcal{J}_\beta(\kappa) \geq \mathcal{J}_\beta(\kappa-1)$, set $\mu = \mu/2$ and go to (b3); otherwise continue;
(b7) if $|\mathcal{J}_\beta(\kappa) - \mathcal{J}_\beta(\kappa-1)|/|\mathcal{J}_\beta(\kappa)| > \tau$, set $\mu = 1.5\mu$ and go to (b1); otherwise stop.

The bulk of the computational costs are found in the backward-in-time solution of the adjoint system in step (b2) and in the forward-in-time solution of the state system in step (b4).

4. Conclusions. In the large eddy simulation without near wall resolution of turbulent flows there occurs three significant closure modeling problems: the interior closure of the subfilter scale stresses, the problem of specifying local boundary conditions for nonlocal flow averages and commutator closure problem. (The last two can be avoided at the price of resolving the turbulent boundary layers.) The commutator closure problem is particularly difficult; to our knowledge so far the only proposed model is that of Das and Moser. We prove herein that the Das Moser commutator closure leads to a well posed problem and show that the global optimizer can be computed through an adjoint problem.

The commutator closure problem is particularly challenging and deserving of much further study.

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