# STABILISATION PARAMETER DETERMINATION FOR THE STOKES EQUATIONS 

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#### Abstract

Parameters for SGS models within the variational multiscale method for the Stokes equations are determined using two different methods. Both linear and nonlinear models are considered. Firstly, optimal parameters are found using a goal-oriented model-constrained technique minimising $L_{2}$ error. Secondly, parameters are obtained using the variational Germano identity. Using the goal-oriented results as reference values, it is shown that the performance of the Germano approach is sensitive to the form of the SGS model.


## 1 Introduction

The variational multiscale method of Hughes et al [1] provides a consistent approach to accounting for the effects of unresolved scales on computed numerical solutions, as well as guidance for the design of models which account for those scales. For simplified equations, exact unresolved-scale (subgrid-scale) models can be derived. These have been used as a guide in the design of models for more complex systems of equations, although this necessarily involves approximations. Consequently, it can be difficult to precisely estimate the parameters of complex subgrid scale (SGS) models, yet these can have a strong influence on the overall performance of the method.

The variational Germano method (VGM), initially developed by Oberai et al [2] seems to be a promising approach to the estimation of such parameters [3, 4]. Yet in the absence of objective reference data, it can be difficult to assess how effective the VGM is for the estimation of parameters on coarse meshes, as competing sources of error are present. Furthermore, it is not always clear which models are the most suitable for use with the VGM.

In this paper we establish objective reference parameters for the multiscale stabilisation of the steady stokes equations using a goal-oriented, modelconstrained optimisation technique. We consider both linear and non-linear subgrid-scale (SGS) models. The optimisation is defined to produce the minimum $L_{2}$ error for a given problem. We also estimate the same parameters
using a VGM for nonlinear models based on the Broyden-Fletcher-GoldfarbShanno algorithm. As the VGM results can differ substantially from optimum values, we investigate the influence of the characteristics of the model on the effectiveness of the VGM approach.

The paper begins with a brief description of a variational-multiscale descretisation of the Stokes equations. Next the goal-oriented model-constrained optimisation technique and variational Germano methods are described in detail. Then results are presented for a simplified linear model, the linear model of Franca et al [5] and the nonlinear model of Taylor et al [6]. In doing so, the correspondence of the results with the mesh-dependent behaviour of the VGM residuals is examined.

## 2 Variational multiscale method

We consider the steady two-dimensional Stokes equations:

$$
\begin{align*}
&-\nabla \cdot\left(2 \nu \nabla^{s} \boldsymbol{u}\right)+\nabla p=\boldsymbol{f} \text { in } \Omega,  \tag{1a}\\
& \nabla \cdot \boldsymbol{u}=0 \text { in } \Omega,  \tag{1b}\\
& \boldsymbol{u}=0 \text { on } \delta \Omega, \quad \int_{\Omega} p d \Omega=0 \tag{1c}
\end{align*}
$$

where $\Omega:=] 0,1[\times] 0,1[$ is the unit square, $\nu$ is the viscosity, and the symmetric velocity gradient is defined as $\nabla^{s} \boldsymbol{u}=\frac{1}{2}\left(\nabla \boldsymbol{u}+\nabla \boldsymbol{u}^{T}\right)$. In the variational multiscale method (VMM), $\boldsymbol{u}$ and $p$ are separated into resolved and unresolved scales such that $\boldsymbol{u}=\boldsymbol{u}^{h}+\boldsymbol{u}^{\prime}$ and $p=p^{h}+p^{\prime}$, with the unresolved scales defined as:

$$
\begin{align*}
\boldsymbol{u}^{\prime}=-\tau_{m} \boldsymbol{R}_{\boldsymbol{m}}, & \boldsymbol{R}_{\boldsymbol{m}}=\nabla p^{h}-\boldsymbol{f}  \tag{2}\\
p^{\prime}=-\tau_{c} R_{c}, & R_{c}=\nabla \cdot u \tag{3}
\end{align*}
$$

Defining $\mathcal{V}^{h}$ and $\mathcal{Q}^{h}$ as spaces of standard bilinear finite-element basis functions with $v \in \mathcal{V}^{h}: v=0$ on $\delta \Omega$ and $v \in \mathcal{Q}^{h}: \int_{\Omega} d \Omega=0$, the variational multiscale formulation of the problem can be written:

$$
\begin{array}{r}
\text { for all } \boldsymbol{w} \in \mathcal{V}^{h} \times V^{h}, q \in \mathcal{Q}^{h} \text { find } \boldsymbol{u}^{h} \in \mathcal{V}^{h} \times V^{h}, p^{h} \in \mathcal{Q}^{h}: \\
\left(\nabla^{s} \boldsymbol{w}, 2 \nu \nabla^{s} \boldsymbol{u}^{h}\right)-\left(\nabla \cdot \boldsymbol{w}, p^{h}\right)+\left(q, \nabla \cdot \boldsymbol{u}^{h}\right)+\left(\nabla \cdot \boldsymbol{w}, \tau_{c} \nabla \cdot \boldsymbol{u}^{h}\right) \\
+\left(\nabla q, \tau_{m}\left(\nabla p^{h}-\boldsymbol{f}\right)\right)=(\boldsymbol{w}, \boldsymbol{f}) \tag{4}
\end{array}
$$

Franca[5] presented linear expressions for the stabilisation parameters $\tau_{m}$ and $\tau_{c}$ by writing the Stokes problem as a steady symmetric advective-diffusive system. Taylor[6] applied nonlinear expressions to a computation of blood flow. In view of the approximations involved, estimates for the coefficients in these models are not precise. We therefore introduce modified definitions allowing the coefficients to be determined by goal-oriented optimisation or the variational Germano method:

Linear model [5]:

$$
\begin{equation*}
\tau_{m}=\frac{c_{1} h^{2}}{24 \sqrt{2} \nu}, \quad \tau_{c}=c_{2} \nu \tag{5}
\end{equation*}
$$

Nonlinear model [6]:

$$
\begin{equation*}
\tau_{m}=\frac{c_{1} h^{2}}{24 \sqrt{2} \nu}, \quad \tau_{c}=\frac{c_{2} h \sqrt{u^{2}+v^{2}}}{4} \tag{6}
\end{equation*}
$$

## 3 Goal-oriented model-constrained optimisation technique

We pose the problem of finding the model coefficients as an optimisation problem that seeks to minimise a specific goal function, subject to the underlying governing equations. We choose the $L_{2}$ norm error of vector $\boldsymbol{V}=\{\boldsymbol{u}, p\}^{T}$ as the goal functional, which is written as

$$
\begin{equation*}
\min _{\boldsymbol{a}, \gamma} \mathcal{G}=\int_{\Omega}\|\boldsymbol{V}-\hat{\boldsymbol{V}}\| d \Omega \tag{7}
\end{equation*}
$$

subject to

$$
\begin{align*}
\left(\nabla^{s} \boldsymbol{w}, 2 \nu \nabla^{s} \boldsymbol{u}^{h}\right)-\left(\nabla \cdot \boldsymbol{w}, p^{h}\right)+\left(q, \nabla \cdot \boldsymbol{u}^{h}\right)+ & \left(\nabla \cdot \boldsymbol{w}, \tau_{c} \nabla \cdot \boldsymbol{u}^{h}\right) \\
& +\left(\nabla q, \tau_{m}\left(\nabla p^{h}-\boldsymbol{f}\right)\right)=(\boldsymbol{w}, \boldsymbol{f}) . \tag{8}
\end{align*}
$$

Where $\hat{\boldsymbol{V}}$ are exact solutions to the Stokes equations, $\boldsymbol{V}$ are solutions obtained multiscale descretisation with unknown model parameters. $\boldsymbol{a}$ represent the nodal values of $\boldsymbol{V}$ at the local node for the element. In this investigation, for which we focus on a 2D Stokes problem, naturally $\boldsymbol{a}=\{a, b, c\}^{T}$ respectively correspond $\boldsymbol{V}=\{u, v, p\}^{T} . \gamma$ represent parametric coefficients $\left\{c_{1}, c_{2}\right\}^{T}$ inside $\tau_{m}$ and $\tau_{c}$.

To find the optimal $\gamma$ we use a procedure similar to [7]. The optimality conditions for the system (7)-(8) can be derived by defining the Lagrangian functional

$$
\begin{align*}
& \mathcal{L}=\mathcal{G}+\boldsymbol{\lambda}\left(\left(\nabla^{s} \boldsymbol{w}, 2 \nu \nabla^{s} \boldsymbol{u}^{h}\right)-\left(\nabla \cdot \boldsymbol{w}, p^{h}\right)+\left(q, \nabla \cdot \boldsymbol{u}^{h}\right)\right. \\
&\left.+\left(\nabla \cdot \boldsymbol{w}, \tau_{c} \nabla \cdot \boldsymbol{u}^{h}\right)+\left(\nabla q, \tau_{m}\left(\nabla p^{h}-\boldsymbol{f}\right)\right)-(\boldsymbol{w}, \boldsymbol{f})\right) \tag{9}
\end{align*}
$$

where $\boldsymbol{\lambda}$ are a vector of Lagrange multipliers (also knows as adjoint state variables) that respectively enforce the momentum conservation equations and the continuity equation. $\boldsymbol{\lambda}=\left\{\lambda_{1}, \lambda_{2}, \lambda_{3}\right\}^{T}$ so that they meet two components of the momentum equations and the continuity equation. We define the solution interpolations within an elements as

$$
\begin{equation*}
u=\sum_{i=1}^{N} a_{i} w 1_{i}, \quad v=\sum_{i=1}^{N} b_{i} w 2_{i}, \quad p=\sum_{i=1}^{N} c_{i} p_{i}, \quad \boldsymbol{w}=\{w 1, w 2, q\}^{T} . \tag{10}
\end{equation*}
$$

Expanding the Lagrange functional yields

$$
\begin{align*}
\mathcal{L}=\mathcal{G}+ & \lambda_{1}\left[2\left(w 1_{x}, u_{x}\right)+\left(w 1_{y}, u_{y}\right)+\left(w 1_{y}, v_{x}\right)-\left(w 1_{x}, p\right)\right. \\
+ & \left.\left(w 1_{x}, \tau_{c}\left(u_{x}+v_{y}\right)\right)-(w 1, f 1)\right]+\lambda_{2}\left[\left(w 2_{x}, u_{y}\right)+\left(w 2_{x}, v_{x}\right)\right. \\
& \left.+2\left(w 2_{y}, v_{y}\right)-\left(w 2_{y}, p\right)+\left(w 2_{y}, \tau_{c}\left(u_{x}+v_{y}\right)\right]-(w 2, f 2)\right) \\
& +\lambda_{3}\left[\left(q,\left(u_{x}+v_{y}\right)\right)+\left(q_{x}, \tau_{m}\left(p_{x}-f 1\right)\right)+\left(q_{y}, \tau_{m}\left(p_{y}-f 2\right)\right)\right], \tag{11}
\end{align*}
$$

where subscripts indicate differentiation with respect to the subscript. The optimality conditions for the system can be obtained by solving the EulerLagrange equations. The Euler-Lagrange equations are derived by taking variations of the Lagrange formulation with respect to the state, adjoint, and coefficient vector variables. Setting the variation of the Lagrange formulation with respect to Lagrange multiplier vector $\boldsymbol{\lambda}$ to zero recovers the state equation (7). Setting the variation of the Lagrange formulation with respect to the state variables $\boldsymbol{a}$ yields the following adjoint equations:

$$
\begin{array}{r}
\frac{\partial \mathcal{L}}{\partial a}=\int_{\Omega} \frac{w 1(u-\hat{u})}{\|\boldsymbol{V}-\hat{\boldsymbol{V}}\|} d \Omega+\lambda_{1}\left(2\left(w 1_{x}, w 1_{x}\right)+\left(w 1_{y}, w 1_{y}\right)+\left(w 1_{x}, \tau_{c} w 1_{x}\right)\right) \\
+\lambda_{2}\left(\left(w 2_{x}, w 1_{y}\right)+\left(w 2_{y}, \tau_{c} w 1_{x}\right)\right)+\lambda_{3}\left(q, w 1_{x}\right)=0 \\
\begin{array}{r}
\frac{\partial \mathcal{L}}{\partial b}=\int_{\Omega} \frac{w 2(v-\hat{v})}{\|\boldsymbol{V}-\hat{\boldsymbol{V}}\|} d \Omega+\lambda_{1}\left(\left(w 1_{y}, w 2_{x}\right)+\left(w 1_{x}, \tau_{c} w 2_{y}\right)\right) \\
+
\end{array} \begin{array}{r}
\lambda_{2}\left(\left(w 2_{x}, w 2_{x}\right)+2\left(w 2_{y}, w 2_{y}\right)+\left(w 2_{y}, \tau_{c} w 2_{y}\right)\right)+\lambda_{3}\left(q, w 2_{y}\right)=0 \\
\frac{\partial \mathcal{L}}{\partial c}=\int_{\Omega} \frac{q(p-\hat{p})}{\|\boldsymbol{V}-\hat{\boldsymbol{V}}\|} d \Omega-\lambda_{1}\left(w 1_{x}, q\right)-\lambda_{2}\left(w 2_{y}, q\right) \\
+\lambda_{3}\left(\left(q_{x}, \tau_{m} q_{x}\right)+\left(q_{y}, \tau_{m} q_{y}\right)\right)=0
\end{array}
\end{array}
$$

Simplifying the adjoint equation system in a matrix form yields the following matrix equations

$$
\left\{\begin{array}{l}
A_{11} \lambda_{1}+A_{12} \lambda_{2}+A_{13} \lambda_{3}=B_{1}  \tag{13}\\
A_{21} \lambda_{1}+A_{22} \lambda_{2}+A_{23} \lambda_{3}=B_{2} \\
A_{31} \lambda_{1}+A_{32} \lambda_{2}+A_{33} \lambda_{3}=B_{3}
\end{array}\right.
$$

Taking the variation of the Lagrange formulation with respect to vector $\gamma$ yields the following formulation

$$
\begin{align*}
& \frac{\partial \mathcal{L}}{\partial c_{1}}=\frac{\partial \mathcal{G}}{\partial c_{1}}+\lambda_{3}\left(\left(q_{x},\left(p_{x}-f 1\right)\right)+\left(q_{y},\left(p_{y}-f 2\right)\right)\right) \frac{\partial \tau_{m}}{\partial c_{1}}=0  \tag{14a}\\
& \frac{\partial \mathcal{L}}{\partial c_{2}}=\frac{\partial \mathcal{G}}{\partial c_{2}}+\lambda_{1}\left(w 1_{x},\left(u_{x}+v_{y}\right)\right) \frac{\partial \tau_{c}}{\partial c_{2}}+\lambda_{2}\left(w 2_{y},\left(u_{x}+v_{y}\right)\right) \frac{\partial \tau_{c}}{\partial c_{2}}=0 \tag{14b}
\end{align*}
$$

The combined system (4), (12) and (14) represents the first-order Karush-Kuhn-Tucker optimality conditions for the optimisation problem (7)-(8).

Instead of solving the constrained optimisation problem (7)-(8) directly, a segregated approach is used in which coefficients in vector $\gamma$ are updated without any other constraints. in another words, $\min _{\boldsymbol{a}, \boldsymbol{\gamma}} \mathcal{G}(\boldsymbol{a}, \boldsymbol{\gamma})$ in (7) is replaced with $\min _{\boldsymbol{a}, \boldsymbol{\gamma}} \mathcal{G}(\boldsymbol{a}(\gamma), \gamma)$, where the dependence of $\boldsymbol{a}$ on $\gamma$ is implicit through the separately updated state equations. The resulting unconstrained optimisation problem is solved by a Truncated Newton method based on a trust region [8]. Specially, a modified conjugate-gradient (CG) method due to Steihaug [9] is used to solve the system of equations arising at each Newton step and globalise the optimality conditions by a trust-region scheme. The first term of the
gradient (14) required by the Steihaug CG is estimated by a finite difference approximation

$$
\begin{equation*}
\frac{\partial \mathcal{G}}{\partial \gamma_{i}}=\frac{\mathcal{G}\left(\gamma_{i}+\epsilon\right)-\mathcal{G}\left(\gamma_{i}\right)}{\epsilon} \tag{15}
\end{equation*}
$$

where $\epsilon$ is a small increment.
The procedure used to compute the gradient can be summarised as follows. Firstly, the state equations are solved to obtain $\boldsymbol{a}$. Secondly, the adjoint equations are solved to determine Lagrange multipliers $\boldsymbol{\lambda}$. Finally, the computed $\boldsymbol{a}$ and $\boldsymbol{\lambda}$ are used to compute the gradient using (14).

In the Steihaug CG algorithm, we approximate the Hessian-vector product using a Taylor expansion instead of evaluating the complete matrix. To estimate the Hessian-vector product, one needs to repeatedly solve the state and adjoint equations with a pair of updated $\tau$ in which coefficients are added by a small increment $\epsilon$ multiplied by the direction. Consequently, the optimisation algorithm requires solutions to a pair of state and adjoint systems at each CG iteration.

## 4 Variational Germano method

Here the variational Germano method (VGM) is also used to find the coefficients, $\boldsymbol{\gamma}$, of the stabilisation parameters appearing in (4). First the VGM is recast into a least-squares residual form for the Stokes' equations, based on the separation of the momentum and continuity equations. Thereafter the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is proposed as a numerical procedure that can minimise the residuals for arbitrary forms of the stabilisation parameters, $\tau_{m}$ and $\tau_{c}$. In the VGM a series of $N$ coarse function spaces, $\mathcal{W}_{h_{i}}$, are defined with corresponding domain partitions, $\mathcal{C}_{h_{i}}$, parametrised by the coarse length scale $h_{i}$. After first obtaining $\boldsymbol{V}^{h}$ by solving (4) with an initial guess for $\boldsymbol{\gamma}$, the respective coarse-scale solutions, $\boldsymbol{V}^{h_{i}}$, are obtained via a projection: $\boldsymbol{V}^{h_{i}}=\mathbb{P}^{h_{i}} \boldsymbol{V}^{h}$. There are a number of choices for the projector. To obtain parameters comparable to the goal-oriented procedure, here the $L_{2}$ projector is used. Using $\boldsymbol{V}^{h_{i}}$ the weak form of the stabilised Stokes' equations can be reconstructed on each $\boldsymbol{W}^{h_{i}}$, i.e.:

$$
\begin{align*}
\left(\nabla^{s} \boldsymbol{w}^{h_{i}}, 2 \nu \nabla^{s} \boldsymbol{u}^{h_{i}}\right) & -\left(\nabla \cdot \boldsymbol{w}^{h_{i}}, p^{h_{i}}\right)+\left(q^{h_{i}}, \nabla \cdot \boldsymbol{u}^{h_{i}}\right)+\left(\nabla \cdot \boldsymbol{w}^{h_{i}}, \tau_{c} \nabla \cdot \boldsymbol{u}^{h_{i}}\right) \\
& +\left(\nabla q^{h_{i}}, \tau_{m}\left(\nabla p^{h_{i}}-\boldsymbol{f}\right)\right)-\left(\boldsymbol{w}^{h_{i}}, \boldsymbol{f}\right)=0, i=1, \ldots, N \tag{16}
\end{align*}
$$

(16) represents an equation for each function in the span of all the $\boldsymbol{w}^{h_{i}}$ and $q$. However, as $\gamma$ are taken to be globally constant coefficients, (16) is instead interpreted globally, i.e. the inner products are taken over all of $\Omega$. This reduces (16) to one equation per coarse function space.

When $\tau_{m}$ and/or $\tau_{c}$ depend nonlinearly on their coefficients, it may not be possible to obtain an analytical solution for $\boldsymbol{\gamma}$ from (16). Therefore a numerical solution procedure would need to be used. In doing so (16) can be assembled from the individual local contributions of the functions spanning $\boldsymbol{w}^{h_{i}}$.

If the local contributions to (16) are sometimes positive and sometimes negative (16) may be globally very small. This makes it seem as if the chosen $\gamma$ satisfies the Germano relations very well, while the local error of the relations
can still be very large. In this case, a different formulation of (16) can be used. Oberai and Wang propose a least-squares formulation of the Germano relations in [2]. This allows a global Germano residual to be assembled without concern for the sign of the local contributions. First it is noted that in (16), $\tau_{m}$ only appears in the continuity equation and $\tau_{c}$ only appears in the momentum equations. It is thus beneficial to use the linear independence of $q^{h_{i}}$ and $\boldsymbol{w}^{h_{i}}$ to separate the continuity and momentum equations into two separate Germano identities:

$$
\begin{gather*}
\left(\nabla^{s} \boldsymbol{w}^{h_{i}}, 2 \nu \nabla^{s} \boldsymbol{u}^{h_{i}}\right)-\left(\nabla \cdot \boldsymbol{w}^{h_{i}}, p^{h_{i}}\right)+\left(\nabla \cdot \boldsymbol{w}^{h_{i}}, \tau_{c} \nabla \cdot \boldsymbol{u}^{h_{i}}\right)-\left(\boldsymbol{w}^{h_{i}}, \boldsymbol{f}\right)=1, \ldots, N  \tag{18}\\
\left(q^{h_{i}}, \nabla \cdot \boldsymbol{u}^{h_{i}}\right)+\left(\nabla q^{h_{i}}, \tau_{m}\left(\nabla p^{h_{i}}-\boldsymbol{f}\right)\right)=0, i=1, \ldots, N \tag{17}
\end{gather*}
$$

Then let $\boldsymbol{w}^{h_{i}}=\sum_{j} \boldsymbol{\phi}_{j}^{i}$ and $q^{h_{i}}=\sum_{j} \psi_{j}^{i}$, where $\boldsymbol{\phi}_{j}^{i}$ and $\psi_{j}^{i}$ are the individual weighting functions in the space $\mathcal{W}^{h_{i}}$. The local residuals of the momentum and continuity Germano identities are then defined as:

$$
\begin{gather*}
r_{j, m}^{i}:=\left(\nabla^{s} \boldsymbol{\phi}_{j}^{i}, 2 \nu \nabla^{s} \boldsymbol{u}^{h_{i}}\right)-\left(\nabla \cdot \boldsymbol{\phi}_{j}^{i}, p^{h_{i}}\right)+\left(\nabla \cdot \boldsymbol{\phi}_{j}^{i}, \tau_{c} \nabla \cdot \boldsymbol{u}^{h_{i}}\right)-\left(\boldsymbol{\phi}_{j}^{i}, \boldsymbol{f}\right)  \tag{19}\\
r_{j, c}^{i}:=\left(\psi_{j}^{i}, \nabla \cdot \boldsymbol{u}^{h_{i}}\right)+\left(\nabla \psi_{j}^{i}, \tau_{m}\left(\nabla p^{h_{i}}-\boldsymbol{f}\right)\right) \tag{20}
\end{gather*}
$$

The global least-squares residuals can then be constructed by summing the squares of the local residuals:

$$
\begin{equation*}
R_{m}:=\sum_{i=1}^{N} \sum_{j}\left(r_{j, m}^{i}\right)^{2}, \quad R_{c}:=\sum_{i=1}^{N} \sum_{j}\left(r_{j, c}^{i}\right)^{2} \tag{21}
\end{equation*}
$$

$\boldsymbol{\gamma}$ is then obtained by finding values that minimise $R_{m}$ and $R_{c}$. The obtained $\boldsymbol{\gamma}$ can be used to compute a new $\boldsymbol{V}^{h}$ which can then be used to repeat the VGM. Repeating this process gives rise to an iterative solution procedure for optimising $\gamma$.

The BFGS algorithm can be used to minimise $R_{m}$ and $R_{c}$ with respect to $\gamma$. Consider the residual $R$ which may represent either $R_{m}$, or $R_{c}$. $R$ is minimised when its gradient with respect to $\gamma$ is zero. The gradient of $R$ can be approximated using a first order Taylor expansion:

$$
\begin{equation*}
\nabla R(\boldsymbol{\gamma}) \approx \nabla R\left(\gamma_{0}\right)+B\left(\gamma_{0}\right)\left(\gamma-\gamma_{0}\right)=0 \tag{22}
\end{equation*}
$$

where $B$ is the Hessian of $R$ with respect to $\boldsymbol{\gamma}$. Replacing $\gamma_{0}$ by $\gamma_{n}$ and $\boldsymbol{\gamma}$ by $\gamma_{n+1}$, the following iterative procedure can be derived:

$$
\begin{equation*}
\boldsymbol{\gamma}_{n+1}=\boldsymbol{\gamma}_{n}-\alpha_{n} B_{n}^{-1} \nabla R\left(\boldsymbol{\gamma}_{n}\right) \tag{23}
\end{equation*}
$$

$\alpha_{n}$ represents a parameter that controls the step length and is obtained, in this paper, from an inexact line-search. $B_{n}$ represents an approximation to the Hessian at step $n$. $B_{n}$ is obtained by first assuming that $B_{0}=I$, i.e. start with the identity matrix and then updated to $B_{n+1}$ according to the following procedure:

$$
\begin{align*}
B_{n+1} & =B_{n}+\frac{y_{n} y_{n}^{T}}{y_{n}^{T} s_{n}}-\frac{B_{n} s_{n} s_{n}^{T} B_{n}}{s_{n}^{T} B_{n} s_{n}} \\
s_{n} & =\alpha_{n}\left(\boldsymbol{\gamma}_{n+1}-\boldsymbol{\gamma}_{n}\right) \\
y_{n} & =\nabla R\left(\boldsymbol{\gamma}_{n+1}\right)-\nabla R\left(\boldsymbol{\gamma}_{n}\right) \tag{24}
\end{align*}
$$

To complete the algorithm it is noted that $\nabla R$ is evaluated using forward finite differences. The full BFGS algorithm is run until $\|\nabla R\|_{L_{2}}<1 \cdot 10^{-7}$.

## 5 Difference between VGM and $L_{2}$ optimality

When using the VGM, with the $L_{2}$ projector, it is implicitly assumed that there is a correspondence between the residuals $R_{m}$ and $R_{c}$ and the $L_{2}$ error. The numerical solution $\boldsymbol{V}^{h}$ implicitly depends on $\vec{c}$ as $\vec{c}$ modifies the PDE that governs $\boldsymbol{V}^{h}$, this dependence can be represented by allowing $\boldsymbol{V}^{h}$ to be a function of $\vec{c}$. The residuals $R_{m}$ and $R_{c}$ both directly depend on $\vec{c}$ and implicitly on $\boldsymbol{V}^{h}(\vec{c})$. Taking into account the necessary dependencies, the $L_{2}$ error could be written in the following functional form:

$$
\begin{equation*}
L_{2} \text { error }:=F_{L_{2}}\left(R_{m}\left(\boldsymbol{V}^{h}(\vec{c}), \vec{c}\right), R_{c}\left(\boldsymbol{V}^{h}(\vec{c}), \vec{c}\right)\right) \tag{25}
\end{equation*}
$$

The $\vec{c}$ that minimises the $L_{2}$ error then must satisfy:

$$
\begin{equation*}
\frac{\mathrm{d} F_{L_{2}}}{\mathrm{~d} \vec{c}}=\frac{\partial F_{L_{2}}}{\partial R_{m}}\left(\frac{\partial R_{m}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}+\frac{\partial R_{m}}{\partial \vec{c}}\right)+\frac{\partial F_{L_{2}}}{\partial R_{c}}\left(\frac{\partial R_{c}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}+\frac{\partial R_{c}}{\partial \vec{c}}\right)=0 \tag{26}
\end{equation*}
$$

which requires:

- $\frac{\partial F_{L_{2}}}{\partial R_{m}}\left(\frac{\partial R_{m}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}+\frac{\partial R_{m}}{\partial \vec{c}}\right)=-\frac{\partial F_{L_{2}}}{\partial R_{c}}\left(\frac{\partial R_{c}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}+\frac{\partial R_{c}}{\partial \vec{c}}\right)$
- or, $\frac{\partial R_{m}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}=-\frac{\partial R_{m}}{\partial \vec{c}}$ and $\frac{\partial R_{c}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}=-\frac{\partial R_{c}}{\partial \vec{c}}$
- or, $\frac{\partial R_{m}}{\partial V^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}=0, \frac{\partial R_{m}}{\partial \vec{c}}=0, \frac{\partial R_{c}}{\partial V^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}}=0$ and $\frac{\partial R_{c}}{\partial \vec{c}}=0$

The last two points are equivalent to $\frac{\mathrm{d} R_{m}}{\mathrm{~d} \stackrel{c}{c}}=0, \frac{\mathrm{~d} R_{c}}{\mathrm{~d} \bar{c}}=0$, i.e. $R_{m}$ and $R_{c}$ must both be globally minimised for the same $\stackrel{\rightharpoonup}{c}$. Currently $\frac{\partial R_{m}}{\partial \vec{c}} \approx 0$ and $\frac{\partial R_{c}}{\partial \vec{c}} \approx 0$ is obtained via the VGM, which is a standard way of solving the VGM relations. However, from (26) it is clear that the current procedure is not sufficient to find the minimum of the $L_{2}$ error. $\frac{\partial R_{m}}{\partial V^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}} \approx 0$ and $\frac{\partial R_{c}}{\partial \boldsymbol{V}^{h}} \frac{\partial \boldsymbol{V}^{h}}{\partial \vec{c}} \approx 0$ is required as well. This is only possible if there is a single $\vec{c}$ that globally minimises $R_{m}$ and $R_{c}$. It will be shown in the subsequent sections that for a number of SGS models used in practice this is not the case. Therefore, in most cases the $\vec{c}$ obtained from the goal-oriented procedure will not be the same as the $\vec{c}$ obtained from the VGM.

In spite of not minimising the $L_{2}$ error, using the VGM may result in a reduction of the $L_{2}$ error when compared to using standard values for $\vec{c}$. The following sections investigate potential indicators for the suitability of an SGS model. To achieve a further reduction in $L_{2}$ error, use would have to be made of adjoint methods to account for the dependence of $F_{L_{2}}$ on $R_{m}$ and $R_{c}$. However, solving the adjoint problem may make the method prohibitively expensive for practical purposes.

## 6 Results and discussion

In this study, (1a) is solved with $\boldsymbol{f}$ defined by manufactured solutions $\sin (4 \pi x) \sin (4 \pi y)$ for each variable. The manufactured solutions are used for the reference solution $\hat{\boldsymbol{V}}$ while computing the L2 norm error. Here bilinear elements are used for the both the velocity and pressure spaces. The model coefficients are found using both the goal-oriented procedure and the VGM. Since the goal-oriented procedure optimises directly in terms of the desired error norm, it can be used to define coefficient reference values. The VGM results, however, are subject to limitations introduced by the approximation of the subgrid scales. In particular to what extent the SGS model simultaneously minimises the VGM residuals, and to what extent its optimal coefficients are independent of mesh size. For the purposes of discussion, we characterise SGS models for the VGM as follows:

1. Concurrent models: have optimal coefficients that minimise $R_{m}, R_{c}$, and $\left\|\mathbb{P}^{h} \boldsymbol{u}-\boldsymbol{u}^{h}\right\|$ simultaneously.
2. Scale-invariant models: have optimal coefficients that are independent of $h$.

Presumably a concurrent, scale-invariant SGS model would likely realise the full potential of the VGM.

## 6.1 $\tau_{m}$ only models

We first consider the linear model (5) with $\tau_{c}=0$, as well as a similar model with an $h$ parameterisation of $\tau_{m}$ :

$$
\begin{equation*}
\left(\tau_{\mathrm{m}} \text { only, } \mathrm{h}^{2}\right): \tau_{m}=c_{1} \frac{h^{2}}{24 \sqrt{2} \nu}, \quad\left(\tau_{\mathrm{m}} \text { only, } \mathrm{h}\right): \tau_{m}=c_{1} \frac{h}{24 \sqrt{2} \nu} \tag{27}
\end{equation*}
$$

Results for $c_{1}$ versus $h$ obtained using the goal-oriented minimisation of $L_{2}$ error are shown in figure 1. The goal-oriented procedure converges uniformly for this case, requiring on average 10 iterations when starting from an initial guess of $c_{1}=1.0$. Clearly the ( $\tau_{m}$ only, $h^{2}$ ) model is scale invariant, while the ( $\tau_{m}$ only, $h$ ) is not. Also shown in figure 1 are the values of $c_{1}$ obtained from the VGM, corresponding to minimums in $R_{c}$. These differ from their goal-oriented counterparts, in particular the ( $\tau_{m}$ only, $h^{2}$ ) model is now scale-variant.

The VGM results are considered in more detail in figure 2, which shows the variation of $R_{m}, R_{c}$, the $L_{2}$ error and $\left\|\mathbb{P}^{h} \boldsymbol{u}-\boldsymbol{u}^{h}\right\|$ with $c_{1}$. For plotting purposes, $R_{m}$ and $R_{c}$ are rescaled to be one when $c_{1}=0$. It is evident that in all cases $\left\|\boldsymbol{u}-\boldsymbol{u}^{h}\right\|_{L_{2}} \approx\left\|\mathbb{P}^{h} \boldsymbol{u}-\boldsymbol{u}^{h}\right\|_{L_{2}}$ and is minimised for the same value of $c_{1}$, which is identical to the value determined by the goal-oriented method. This shows that for these cases, $L_{2}$ optimality is equivalent to minimising the projected error. For both definitions of $\tau_{m}$ however, the $c_{1}$ obtained from minimising $R_{c}$ does not correspond to the value that minimises either $R_{m}$ or $\left\|\mathbb{P}^{h} \boldsymbol{u}-\boldsymbol{u}^{h}\right\|$. Therefore neither $\tau_{m}$ is concurrent and information of the adjoint problem is needed to minimise the $L_{2}$ error. It is further clear that a scaleinvariant SGS model may not retain its scale-invariance when calibrated with the VGM.


Figure 1: $c_{1}$ versus $h$. Left: $\left(\tau_{m}\right.$ only, $\left.h^{2}\right)$, right: $\left(\tau_{m}\right.$ only, $\left.h\right)$.


Figure 2: Plot of $R_{m}, R_{c}, L_{2}$ error and $\left\|\mathbb{P}^{h} u-u^{h}\right\|$ for different value of $c_{1}$ for the $\left(\tau_{m}\right.$ only, $\left.h^{2}\right)$ and ( $\tau_{m}$ only, $h$ ) models with $h=1 / 12$ and $h=1 / 24$.

### 6.2 Models with both $\tau_{m}$ and $\tau_{c}$

We now consider the more conventional linear (5) and nonlinear (6) models which use both $\tau_{m}$ and $\tau_{c}$. Fig (3) shows contours of the $L_{2}$ error versus $c_{1}$ and $c_{2}$ for the manufactured solution on a uniform mesh of $32 \times 32$ elements. These are the two-dimensional counterparts of the $\left\|\boldsymbol{u}-\boldsymbol{u}^{h}\right\|_{L_{2}}$ curves of figure 2. Interestingly, the linear model exhibits more complex behaviour than the nonlinear one. Two minimums are present for the linear model, which also appears to be less sensitive to the value of $c_{1}$. Optimal coefficients obtained with the goal-oriented optimisation are compared to those obtained with the VGM in figure 4. The coefficients determined by the VGM vary widely in this range. Only the goal-oriented $c_{1}$ value is relatively scale-invariant, while the other coefficients show wide variation but possibly convergence for smaller $h$.


Figure 3: L2 error norm versus $\boldsymbol{\gamma}$. Left: linear stabilisation parameters, right: nonlinear stabilisation parameters.


Figure 4: $\tau$ coefficients versus $h$. Left: linear stabilisation parameters, right: nonlinear stabilisation parameters.

Figure 5 shows the behaviour of $R_{c}$ and $R_{m}$ for the linear model. These indicate that the model lacks both concurrency and scale invariance in the $h$ range of greatest interest. A similar conclusion can be obtained by examining $R_{c}$ and $R_{m}$ for the nonlinear model. Thus information about the adjoint problem is again needed to be able to minimise the $L_{2}$ error. For the mesh with size $h=1 / 24$, the values of $c_{1}$ and $c_{2}$ obtained for the linear $\tau$ s are closer to the minimums of $R_{c}$ and $R_{m}$ than those obtained by the goal-oriented procedure. This is coherent with (26) in that obtaining coefficients that minimise the $L_{2}$ error may not necessarily require a minimisation of $R_{c}$ and $R_{m}$. Figure 6 shows the consequence of the differences between the VGM and goal-oriented method. Although the VGM results converge uniformly with mesh size, the value of the VGM errors can be more than an order of magnitude greater than those of their goal-oriented counterparts. Note that the goal-oriented values for the non-linear model are also superior to those suggested in [6]. Furthermore, while neither the linear, or nonlinear $\tau \mathrm{s}$ are scale-invariant or concurrent, the nonlinear $\tau$ s produce vastly lower $L_{2}$ errors than the linear $\tau \mathrm{s}$ when used with the VGM. This makes it clear that when a model lacks concurrency, scale-invariance may not be required for it to work well with the VGM.


Figure 5: $R_{c}$ and $R_{m}$ contours for the linear model


Figure 6: $L_{2}$ error of models which use both $\tau_{m}$ and $\tau_{c}$.

## 7 Conclusions

Parameters of a variational multiscale model for the Stokes equations have been determined using a goal-oriented procedure and the VGM. In this context the goal-oriented procedure provides exact reference values, while the VGM represents an approach which can be used in practice. Differences in the goal criteria of the goal-oriented method and the VGM, with $L_{2}$ projection, show that the VGM will not necessarily produce coefficient values that minimise the $L_{2}$ error. The results also demonstrate that the quality of the parameters predicted by the VGM are strongly affected by the form of the SGS model. Specifically, when a model lacks concurrency in the minimisation of its VGM
residuals, or when a model is scale variant, it becomes difficult to realise its full potential using the VGM. In the absence of concurrency the adjoint problem relating the $L_{2}$ error to the VGM residuals must be solved to find SGS model coefficients that minimise the $L_{2}$ error. Furthermore a scale-variant non-concurrent model may still perform well with the VGM. The results also indicate that it may be possible to assess the suitability of a particular model for the VGM by examining the variation of the VGM residuals with mesh size.

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