

# Variational multiscale finite element formulation for computational fluid dynamics

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April 18, 2020

## 1 Theory

### 1.1 Fluid mechanics

Given is a domain  $\Omega$  with a piecewise continuous boundary  $\Gamma = \partial\Omega$  within which a Newtonian incompressible fluid flow is found. The unknown fields are the time dependent velocity and pressure fields denoted as  $\mathbf{u}$  and  $p$ , respectively. The fluid's density  $\rho$  and kinematic viscosity  $\mu$  are assumed to be constant. The so-called dynamic viscosity of the flow is defined as the ratio of the kinematic viscosity divided by the fluid density  $\nu = \mu/\rho$ . Moreover, assumed is also that the fluid flow is subject to body forces (e.g. gravitational forces)  $\mathbf{f}$ . The velocity and/or pressure field are prescribed to a fixed value  $\bar{\mathbf{u}}$  and  $\bar{p}$ , respectively, along a portion of the domain's boundary known as the inlet (Dirichlet) boundary  $\Gamma_d \subset \Gamma$ . The fluid traction vector along a cut  $\gamma \subset \bar{\Omega}$  with outward normal  $\mathbf{n}$  is given by,

$$\mathbf{t} = -p\mathbf{n} + \mathbf{n} \cdot \nu \nabla^s \mathbf{u} , \quad (1)$$

where  $\nabla^s$  stands for the symmetric gradient operator namely,  $\nabla^s = 1/2 (\nabla + \nabla^t)$ . Moreover  $p$  is expressed in Nm/Kg since it is normalized by the fluid density, meaning that the actual pressure is obtained by  $\tilde{p} = \rho p$ . The domain  $\Omega$  is also assumed to be moving with a given velocity  $\mathbf{u}_d$  independently of the fluid flow. Then, accordingly to the *Arbitrary Lagrangian-Eulerian* description of motion, the inertial forces are given by means of the material derivative  $D(\bullet) = (\dot{\bullet}) + (\mathbf{u} - \mathbf{u}_d) \cdot \nabla(\bullet)$ , where  $(\dot{\bullet}) = \partial(\bullet)/\partial t$  stands for the time derivative. Accordingly, the strong formulation of the transient incompressible Navier-Stokes problem writes; Find the velocity and pressure field  $\mathbf{u} \in \mathbf{C}^2(\Omega)$  and  $p \in C^1(\Omega)$ , respectively, such that,

$$\dot{\mathbf{u}} - \nu \Delta \mathbf{u} + (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} + \nabla p = \mathbf{f} \quad \text{in } \Omega , \quad (2a)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega , \quad (2b)$$

$$\mathbf{u} = \bar{\mathbf{u}} \quad \text{on } \Gamma_d , \quad (2c)$$

$$p = \bar{p} \quad \text{on } \Gamma_d , \quad (2d)$$

$$\mathbf{t} = \bar{\mathbf{t}} \quad \text{on } \Gamma_n , \quad (2e)$$

where  $\bar{\mathbf{t}}$  stands for the applied traction vector on the outlet (Neumann) boundary  $\Gamma_n \subset \Gamma$ . Regarding the symbols in Eq. (2),  $\Delta(\bullet) = \partial^2(\bullet)/\partial X_1^2 + \partial^2(\bullet)/\partial X_2^2$  stands for the Laplace second-order operator with respect to  $\mathbf{X} = X_\alpha \mathbf{e}_\alpha \in \Omega$  where the Einstein's summation convention over repeated indices is assumed, whenever not otherwise stated, and where Greek and Latin indices range from 1 to 2 and from 1 to 3, respectively.

### 1.2 Variational multiscale stabilization of the weak formulation

Multiplying Eqs. (2a) and (2b) by test functions  $\delta \mathbf{u}$  and  $\delta p$ , respectively, integrating over  $\Omega$ , performing integration by parts and applying the boundary conditions yields the following variational formulation; Find  $\mathbf{u} \in \mathcal{H}^1(\Omega)$  and  $p \in \mathcal{L}^2(\Omega)$  such that,

$$\begin{aligned} \langle \delta \mathbf{u}, \dot{\mathbf{u}} \rangle_{0,\Omega} + \langle \nu \nabla \delta \mathbf{u}, \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \delta \mathbf{u}, (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} - \langle \delta \mathbf{u}, p \rangle_{0,\Omega} - \langle \delta p, \nabla \cdot \mathbf{u} \rangle_{0,\Omega} = \\ \langle \delta \mathbf{u}, \mathbf{f} \rangle_{0,\Omega} + \langle \delta \mathbf{u}, \bar{\mathbf{t}} \rangle_{0,\Gamma_c} , \end{aligned} \quad (3)$$

for all  $\delta \mathbf{u} \in \mathcal{H}^1(\Omega)$  and all  $\delta p \in \mathcal{L}^2(\Omega)$ , where  $\langle \mathfrak{T}, \mathfrak{T}' \rangle_{0,\Omega} = \int_{\Omega} \mathfrak{T}_{\alpha_1 \dots \alpha_m} \mathfrak{T}'_{\alpha_1 \dots \alpha_m} d\Omega$  stands for the  $\mathcal{L}^2$ -norm in  $\Omega$  for any pair of equal order tensors  $\mathfrak{T}, \mathfrak{T}' \in \mathfrak{S}^m$ . The discrete form of variational formulation in Eq. (3) has a unique solution given that the so-called *Ladyzhenskaya-Babuška-Brezzi* (LBB) or *inf-sup* condition is satisfied by the discrete spaces. It has been shown that for specific pairs of the  $\mathbf{u}$ - $p$  discretization, such as p1-p0, this is satisfied but for equal order interpolations of the velocity and pressure fields this is not the case. This in turn leads into nearly singular matrices and oscillatory (checkerboard patten) pressure fields.

Herein the so-called *Variational Multi-Scale* (VMS) stabilization [HFMQ98] with the *Algebraic Sub-Grid Scales* (ASGS) projection [Cod01] of variational formulation in Eq. (3) is employed. Accordingly, the unknown fields are comprised by two parts, the coarse or resolvable scale fields and the fine or subscale fields. The former is resolvable within the finite element discretization whereas the latter is not. Therefore, the subscales are modeled by projecting the residuals of the Navier-Stokes Eqs. (2a) and (2b) onto the subscales. Let  $\tilde{\mathcal{L}} : \mathbf{C}^2(\Omega) \times C^1(\Omega) \rightarrow \mathbb{R}^3$  be the differential operator of the Navier-Stokes Eqs.(2a), (2b), namely,

$$\tilde{\mathcal{L}} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \dot{\mathbf{u}} - \nu \Delta \mathbf{u} + (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} + \nabla p \\ \nabla \cdot \mathbf{u} \end{bmatrix}, \quad (4)$$

then the residual form of the Navier-Stokes equations can be written as,

$$\tilde{\mathcal{R}}(\mathbf{u}, p) = \tilde{\mathcal{L}} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} - \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix}. \quad (5)$$

The Picard-linearized steady-state adjoint operator of the Navier-Stokes equations  $\tilde{\mathcal{L}}^* : \mathbf{C}^2(\Omega) \times C^1(\Omega) \rightarrow \mathbb{R}^3$  writes,

$$\tilde{\mathcal{L}}^* \begin{bmatrix} \mathbf{u}; \delta \mathbf{u} \\ \delta p \end{bmatrix} = \begin{bmatrix} -\nu \Delta \delta \mathbf{u} - (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \delta \mathbf{u} - \nabla \delta p \\ -\nabla \cdot \delta \mathbf{u} \end{bmatrix}, \quad (6)$$

for a given velocity field  $\mathbf{u}$  of the primal solution. Given also a stabilization second order tensor  $\boldsymbol{\tau} \in \mathfrak{S}^2$ , the VMS-stabilized version of variational formulation in Eq. (3) becomes,

$$\begin{aligned} \left\langle \delta \mathbf{u}, \frac{\partial \mathbf{u}}{\partial t} \right\rangle_{0,\Omega} + \langle \nu \nabla \delta \mathbf{u}, \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \delta \mathbf{u}, (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} - \langle \delta \mathbf{u}, \nabla p \rangle_{0,\Omega} - \langle \delta p, \nabla \cdot \mathbf{u} \rangle_{0,\Omega} - \\ - \left\langle \tilde{\mathcal{L}}^* \begin{bmatrix} \mathbf{u}; \delta \mathbf{u} \\ \delta p \end{bmatrix}, \boldsymbol{\tau} \cdot \tilde{\mathcal{R}}(\mathbf{u}, p) \right\rangle_{0,\Omega} = \langle \delta \mathbf{u}, \mathbf{f} \rangle_{0,\Omega} + \langle \delta \mathbf{u}, \bar{\mathbf{t}} \rangle_{0,\Gamma_c}. \end{aligned} \quad (7)$$

The stabilization tensor  $\boldsymbol{\tau} = \tau_{\alpha\beta} \mathbf{e}_1 \otimes \mathbf{e}_2$  is chosen diagonal, that is,  $\tau_{12} = \tau_{21} = 0$ ,  $\tau_{11} = \tau_m$  and  $\tau_{22} = \tau_c$ . In this way, the VMS-stabilized variational formulation in Eq. (7) becomes,

$$\begin{aligned} \langle \delta \mathbf{u}, \dot{\mathbf{u}} \rangle_{0,\Omega} - \langle \Delta \delta \mathbf{u}, \nu \tau_m \dot{\mathbf{u}} \rangle_{0,\Omega} - \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \delta \mathbf{u}, \tau_m \dot{\mathbf{u}} \rangle_{0,\Omega} - \langle \nabla \delta p, \tau_m \dot{\mathbf{u}} \rangle_{0,\Omega} + \langle \nabla \delta \mathbf{u}, \nu \nabla \mathbf{u} \rangle_{0,\Omega} + \\ \langle \delta \mathbf{u}, (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} - \langle \delta \mathbf{u}, \nabla p \rangle_{0,\Omega} - \langle \delta p, \nabla \cdot \mathbf{u} \rangle_{0,\Omega} - \langle \Delta \delta \mathbf{u}, \nu^2 \tau_m \Delta \mathbf{u} \rangle_{0,\Omega} - \\ \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \delta \mathbf{u}, \nu \tau_m \Delta \mathbf{u} \rangle_{0,\Omega} - \langle \nabla \delta p, \nu \tau_m \Delta \mathbf{u} \rangle_{0,\Omega} + \langle \Delta \delta \mathbf{u}, \nu \tau_m (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} + \\ \langle \nabla \delta p, \tau_m (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \Delta \delta \mathbf{u}, \nu \tau_m \nabla p \rangle_{0,\Omega} + \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \delta \mathbf{u}, \tau_m \nabla p \rangle_{0,\Omega} + \\ \langle \nabla \delta p, \tau_m \nabla p \rangle_{0,\Omega} + \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \delta \mathbf{u}, \tau_m (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \nabla \cdot \delta \mathbf{u}, \tau_c \nabla \cdot \mathbf{u} \rangle_{0,\Omega} = \\ \langle \Delta \delta \mathbf{u}, \nu \tau_m \mathbf{f} \rangle_{0,\Omega} + \langle \mathbf{u} \cdot \nabla \delta \mathbf{u}, \tau_m \mathbf{f} \rangle_{0,\Omega} + \langle \nabla \delta p, \tau_m \mathbf{f} \rangle_{0,\Omega} + \langle \delta \mathbf{u}, \mathbf{f} \rangle_{0,\Omega} + \langle \delta \mathbf{u}, \bar{\mathbf{t}} \rangle_{0,\Gamma_c}. \end{aligned} \quad (8)$$

## 2 Spatial discretization

Assumed is that the velocity and pressure fields is discretized with the standard linear *Finite Element Method* (FEM) on triangles. Employing the Buvnon-Galerkin FEM, the unknown velocity/pressures fields  $(\mathbf{u}, p)$  and their variation  $(\delta \mathbf{u}, \delta p)$  are discretized using the same basis functions  $(\boldsymbol{\varphi}_i, \phi_i)$ , that is,

$$\begin{bmatrix} \mathbf{u}_h \\ p_h \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} \varphi_i & 0 & 0 \\ 0 & \varphi_i & 0 \\ 0 & 0 & \varphi_i \end{bmatrix} \begin{bmatrix} \hat{u}_{2i-1} \\ \hat{u}_{2i} \\ \hat{p}_i \end{bmatrix}, \quad (9a)$$

$$\begin{bmatrix} \delta \mathbf{u}_h \\ \delta p_h \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} \varphi_i & 0 & 0 \\ 0 & \varphi_i & 0 \\ 0 & 0 & \varphi_i \end{bmatrix} \begin{bmatrix} \delta \hat{u}_{2i-1} \\ \delta \hat{u}_{2i} \\ \delta \hat{p}_i \end{bmatrix}, \quad (9b)$$

where  $\varphi_i$  are the linear basis functions at the element's parametric space. Let,

$$\varphi_i = \varphi_{\text{mod } \frac{i}{2} \mathbf{e}_{\text{mod } \frac{i+1}{2} + 1}}, \quad (10)$$

be the vector-valued basis function for the discretization of the velocity field along  $\text{mod}((i+1)/2)+1$ -Cartesian direction, where  $i = 1, \dots, 2n$  and  $\mathbf{e}_\alpha$  stands for the Cartesian base vector along the  $\alpha$ -Cartesian direction. Accordingly,  $(\hat{u}_i, \hat{p}_i)$  and  $(\delta \hat{u}_i, \delta \hat{p}_i)$  stand for the *Degrees of Freedom* (DOFs) of the unknown and the test fields, respectively, and  $n \in \mathbb{N}$  is the number of nodes in the mesh. Subscript  $h$  indicates then the smallest element length size within the computational mesh.

Substituting Eq. (9b) in Eq. (8) and taking the variation with respect to DOFs  $(\delta \hat{u}_i, \delta \hat{p}_i)$  the following discrete residual systems of equations  $\hat{\mathbf{R}}(\mathbf{u}, \mathbf{p})$  and  $\hat{\mathcal{R}}(\mathbf{u}, \mathbf{p})$ , respectively, are obtained,

$$\begin{aligned} \hat{R}_i(\mathbf{u}, \mathbf{p}) &= \frac{\partial(8)}{\partial \delta \hat{u}_i} = \langle \varphi_i, \dot{\mathbf{u}} \rangle_{0,\Omega} - \langle \Delta \varphi_i, \nu \tau_m \dot{\mathbf{u}} \rangle_{0,\Omega} - \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \dot{\mathbf{u}} \rangle_{0,\Omega} + \\ &\quad \langle \nabla \varphi_i, \nu \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \varphi_i \cdot (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} - \langle \varphi_i, \nabla p \rangle_{0,\Omega} - \langle \Delta \varphi_i, \nu^2 \tau_m \Delta \mathbf{u} \rangle_{0,\Omega} - \\ &\quad \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \varphi_i, \nu \tau_m \Delta \mathbf{u} \rangle_{0,\Omega} + \langle \Delta \varphi_i, \nu \tau_m (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \Delta \varphi_i, \nu \tau_m \nabla p \rangle_{0,\Omega} + \\ &\quad \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \nabla p \rangle_{0,\Omega} + \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} + \\ &\quad \langle \nabla \cdot \varphi_i, \tau_c \nabla \cdot \mathbf{u} \rangle_{0,\Omega} - \langle \Delta \varphi_i, \nu \tau_m \mathbf{f} \rangle_{0,\Omega} - \langle (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \mathbf{f} \rangle_{0,\Omega} - \\ &\quad \langle \varphi_i, \mathbf{f} \rangle_{0,\Omega} - \langle \varphi_i, \bar{\mathbf{t}} \rangle_{0,\Gamma_c}, \end{aligned} \quad (11a)$$

$$\begin{aligned} \hat{\mathcal{R}}_i(\mathbf{u}, \mathbf{p}) &= \frac{\partial(8)}{\partial \delta \hat{p}_i} = - \langle \nabla \varphi_i, \tau_m \dot{\mathbf{u}} \rangle_{0,\Omega} - \langle \varphi_i, \nabla \cdot \mathbf{u} \rangle_{0,\Omega} - \langle \nabla \varphi_i, \nu \tau_m \Delta \mathbf{u} \rangle_{0,\Omega} + \\ &\quad \langle \nabla \varphi_i, \tau_m (\mathbf{u} - \mathbf{u}_d) \cdot \nabla \mathbf{u} \rangle_{0,\Omega} + \langle \nabla \varphi_i, \tau_m \nabla p \rangle_{0,\Omega} - \langle \nabla \varphi_i, \tau_m \mathbf{f} \rangle_{0,\Omega}. \end{aligned} \quad (11b)$$

Applying the approximations in Eq. (9a) into residual Eqs. (11a) and (11b) one obtains the following matrix-vector expressions for the dynamic residual equations,

$$\begin{bmatrix} \hat{\mathbf{R}}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) \\ \hat{\mathcal{R}}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) \end{bmatrix} = \begin{bmatrix} \mathbf{M}(\hat{\mathbf{u}}) & \mathbf{0} \\ \mathcal{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \dot{\hat{\mathbf{u}}} \\ \dot{\hat{\mathbf{p}}} \end{bmatrix} + \begin{bmatrix} \bar{\mathbf{R}}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) \\ \bar{\mathcal{R}}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) \end{bmatrix} - \begin{bmatrix} \hat{\mathbf{F}}(\hat{\mathbf{u}}) \\ \hat{\mathcal{F}} \end{bmatrix}, \quad (12)$$

where  $\hat{\mathbf{u}}$  and  $\hat{\mathbf{p}}$  stand for the complete vectors of velocity and pressure DOFs, that is,

$$\hat{\mathbf{u}} = \begin{bmatrix} \hat{u}_1 & \cdots & \hat{u}_{2n} \end{bmatrix}, \quad (13a)$$

$$\hat{\mathbf{p}} = \begin{bmatrix} \hat{p}_1 & \cdots & \hat{p}_n \end{bmatrix}, \quad (13b)$$

and  $\dot{\hat{\mathbf{u}}}$  and  $\dot{\hat{\mathbf{p}}}$  their time derivatives. Mass matrices  $\mathbf{M}(\hat{\mathbf{u}})$ ,  $\mathcal{M}$ , steady-state residual vectors  $\bar{\mathbf{R}}(\hat{\mathbf{u}}, \hat{\mathbf{p}})$ ,  $\bar{\mathcal{R}}(\hat{\mathbf{u}}, \hat{\mathbf{p}})$  and force vectors  $\hat{\mathbf{F}}(\hat{\mathbf{u}})$ ,  $\hat{\mathcal{F}}$  in Eq. (12) are defined as follows,

$$M_{ij}(\hat{\mathbf{u}}) = \langle \varphi_i, \varphi_j \rangle_{0,\Omega} - \langle \Delta \varphi_i, \nu \tau_m \varphi_j \rangle_{0,\Omega} - \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \varphi_j \rangle_{0,\Omega}, \quad (14a)$$

$$\mathcal{M}_{ij} = - \langle \nabla \varphi_i, \tau_m \varphi_j \rangle_{0,\Omega}, \quad (14b)$$

$$\begin{aligned} \bar{R}_i(\hat{\mathbf{u}}, \hat{\mathbf{p}}) = & \langle \nabla \varphi_i, \nu \nabla \mathbf{u}_h \rangle_{0,\Omega} + \langle \varphi_i, (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \mathbf{u}_h \rangle_{0,\Omega} - \langle \varphi_i, \nabla p_h \rangle_{0,\Omega} - \\ & \langle \Delta \varphi_i, \nu^2 \tau_m \Delta \mathbf{u}_h \rangle_{0,\Omega} - \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \nu \tau_m \Delta \mathbf{u}_h \rangle_{0,\Omega} + \\ & \langle \Delta \varphi_i, \nu \tau_m (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \mathbf{u}_h \rangle_{0,\Omega} + \langle \Delta \varphi_i, \nu \tau_m \nabla p_h \rangle_{0,\Omega} + \\ & \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \nabla p_h \rangle_{0,\Omega} + \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \mathbf{u}_h \rangle_{0,\Omega} + \\ & \langle \nabla \cdot \varphi_i, \tau_c \nabla \cdot \mathbf{u}_h \rangle_{0,\Omega} \end{aligned} \quad (14c)$$

$$\begin{aligned} \bar{\mathcal{R}}_i(\hat{\mathbf{u}}, \hat{\mathbf{p}}) = & - \langle \varphi_i, \nabla \cdot \mathbf{u}_h \rangle_{0,\Omega} - \langle \nabla \varphi_i, \nu \tau_m \Delta \mathbf{u}_h \rangle_{0,\Omega} + \langle \nabla \varphi_i, \tau_m (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \mathbf{u}_h \rangle_{0,\Omega} + \\ & \langle \nabla \varphi_i, \tau_m \nabla p_h \rangle_{0,\Omega}, \end{aligned} \quad (14d)$$

$$\hat{F}_i(\hat{\mathbf{u}}) = \langle \Delta \varphi_i, \nu \tau_m \mathbf{f} \rangle_{0,\Omega} + \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \mathbf{f} \rangle_{0,\Omega} + \langle \varphi_i, \mathbf{f} \rangle_{0,\Omega} + \langle \varphi_i, \bar{\mathbf{t}} \rangle_{0,\Gamma_c}, \quad (14e)$$

$$\hat{\mathcal{F}}_i = \langle \tau_m \nabla \varphi_i, \mathbf{f} \rangle_{0,\Omega}, \quad (14f)$$

where  $\mathbf{u}_h$  and  $p_h$  is the numerical approximation using the finite element method as per Eqs. (13).

### 3 Time discretization

#### 3.1 Bossak time integration scheme

Within the so-called Bossak time integration scheme [WBZ80], given two reals  $\alpha_b, \gamma_b \in \mathbb{R}$  and a time discretization with time step  $dt = t_{\hat{n}+1} - t_{\hat{n}}$ , the following approximation of residual equations in Eq. (12) are made,

$$\begin{aligned} \begin{bmatrix} \hat{\mathbf{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \\ \hat{\mathcal{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \end{bmatrix} = & (1 - \alpha_b) \begin{bmatrix} \mathbf{M}(\hat{\mathbf{u}}_{\hat{n}+1}) & \mathbf{0} \\ \mathcal{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \dot{\hat{\mathbf{u}}}_{\hat{n}+1} \\ \dot{\hat{\mathbf{p}}}_{\hat{n}+1} \end{bmatrix} + \alpha_b \begin{bmatrix} \mathbf{M}(\hat{\mathbf{u}}_{\hat{n}}) & \mathbf{0} \\ \mathcal{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \dot{\hat{\mathbf{u}}}_{\hat{n}} \\ \dot{\hat{\mathbf{p}}}_{\hat{n}} \end{bmatrix} + \\ & \begin{bmatrix} \bar{\mathbf{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \\ \bar{\mathcal{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \end{bmatrix} - \begin{bmatrix} \hat{\mathbf{F}}_{\hat{n}+1}(\hat{\mathbf{u}}_{\hat{n}+1}) \\ \hat{\mathcal{F}}_{\hat{n}+1} \end{bmatrix}, \end{aligned} \quad (15a)$$

$$\begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}+1} \\ \hat{\mathbf{p}}_{\hat{n}+1} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}} \\ \hat{\mathbf{p}}_{\hat{n}} \end{bmatrix} + dt (1 - \gamma_b) \begin{bmatrix} \dot{\hat{\mathbf{u}}}_{\hat{n}} \\ \dot{\hat{\mathbf{p}}}_{\hat{n}} \end{bmatrix} + dt \gamma_b \begin{bmatrix} \dot{\hat{\mathbf{u}}}_{\hat{n}+1} \\ \dot{\hat{\mathbf{p}}}_{\hat{n}+1} \end{bmatrix}. \quad (15b)$$

The subscript  $\hat{n}$  indicates the time instance at which the quantities are evaluated, that is for example  $\hat{\mathbf{u}}_{\hat{n}} = \hat{\mathbf{u}}(t_{\hat{n}})$ . Solving Eqs. (15b) for the time derivatives of the unknown fields at the current time instance  $t_{\hat{n}+1}$  and substituting them into (15a) one arrives at a nonlinear residual equation which is to be solved for the pair  $(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1})$  at the current time instance, namely,

$$\begin{aligned} \begin{bmatrix} \hat{\mathbf{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \\ \hat{\mathcal{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \end{bmatrix} = & \frac{1 - \alpha_b}{\gamma_b} \begin{bmatrix} \mathbf{M}(\hat{\mathbf{u}}_{\hat{n}+1}) & \mathbf{0} \\ \mathcal{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}+1} \\ \hat{\mathbf{p}}_{\hat{n}+1} \end{bmatrix} + \begin{bmatrix} \bar{\mathbf{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \\ \bar{\mathcal{R}}(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1}) \end{bmatrix} - \\ & \frac{1 - \alpha_b}{dt \gamma_b} \begin{bmatrix} \mathbf{M}(\hat{\mathbf{u}}_{\hat{n}+1}) & \mathbf{0} \\ \mathcal{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}} \\ \hat{\mathbf{p}}_{\hat{n}} \end{bmatrix} - \frac{1 - \alpha_b - \gamma_b}{\gamma_b} \begin{bmatrix} \mathbf{M}(\hat{\mathbf{u}}_{\hat{n}+1}) & \mathbf{0} \\ \mathcal{M} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \dot{\hat{\mathbf{u}}}_{\hat{n}} \\ \dot{\hat{\mathbf{p}}}_{\hat{n}} \end{bmatrix} - \\ & \begin{bmatrix} \hat{\mathbf{F}}_{\hat{n}+1}(\hat{\mathbf{u}}_{\hat{n}+1}) \\ \hat{\mathcal{F}}_{\hat{n}+1} \end{bmatrix}. \end{aligned} \quad (16)$$

As equation system in Eq. (16) is highly nonlinear on  $(\hat{\mathbf{u}}_{\hat{n}+1}, \hat{\mathbf{p}}_{\hat{n}+1})$ , it is not fully linearized but only the actual convection term in Eq. (7) is exactly linearized. For all other terms a Picard linearization is assumed, see also in [Cod01]. Let  $(\hat{\mathbf{u}}_{\hat{n},\hat{i}}, \hat{\mathbf{p}}_{\hat{n},\hat{i}})$  be the solution at time step  $\hat{n}$  and nonlinear iteration  $\hat{i}$ . Within the employed quasi-Newton linearization, for all the terms which depend on  $(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}})$  but the actual convection term, the Picard linearization reads,

$$\begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}+1,0} \\ \hat{\mathbf{p}}_{\hat{n}+1,0} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}} \\ \hat{\mathbf{p}}_{\hat{n}} \end{bmatrix} \quad (17a)$$

$$\begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}+1,\hat{i}} \\ \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{u}}_{\hat{n}+1,\hat{i}-1} \\ \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}-1} \end{bmatrix}, \quad \forall \hat{i} \geq 1 \quad (17b)$$

where  $(\hat{\mathbf{u}}_{\hat{n}}, \hat{\mathbf{p}}_{\hat{n}})$  stands for the converged solution at time instance  $t_{\hat{n}}$  and  $(\hat{\mathbf{u}}_{\hat{n}+1,0}, \hat{\mathbf{p}}_{\hat{n}+1,0})$  stands for the initial guess of the quasi-Newton iterative procedure at time instance  $t_{\hat{n}+1}$ . Therefore, the quasi-Newton linearization of residual equations in Eq. (16) leads to the following set of iterations,

$$\left( \frac{1 - \alpha_b}{\gamma_b} \mathbf{M}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}) + \begin{bmatrix} \mathbf{K}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}}) & \mathcal{C}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}}) \\ \mathfrak{C}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}}) & \mathcal{K}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}}) \end{bmatrix} \right) \begin{bmatrix} \Delta_{\hat{n}+1,\hat{i}} \hat{\mathbf{u}} \\ \Delta_{\hat{n}+1,\hat{i}} \hat{\mathbf{p}} \end{bmatrix} = - \begin{bmatrix} \hat{\mathbf{R}}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}}) \\ \hat{\mathcal{R}}(\hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}, \hat{\mathbf{p}}_{\hat{n}+1,\hat{i}}) \end{bmatrix}, \quad (18)$$

where  $\Delta_{\hat{n}+1,\hat{i}} \hat{\mathbf{u}} = \hat{\mathbf{u}}_{\hat{n}+1,\hat{i}+1} - \hat{\mathbf{u}}_{\hat{n}+1,\hat{i}}$ . Matrices  $\mathbf{K}(\hat{\mathbf{u}}, \hat{\mathbf{p}})$ ,  $\mathcal{C}(\hat{\mathbf{u}}, \hat{\mathbf{p}})$ ,  $\mathfrak{C}(\hat{\mathbf{u}}, \hat{\mathbf{p}})$  and  $\mathcal{K}(\hat{\mathbf{u}}, \hat{\mathbf{p}})$  are defined as follows,

$$K_{ij}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) = \frac{\partial \bar{R}_i(\hat{\mathbf{u}}, \hat{\mathbf{p}})}{\partial \hat{u}_j} = \langle \nabla \varphi_i, \nu \nabla \varphi_j \rangle_{0,\Omega} + \langle \varphi_i, \varphi_j \cdot \nabla \mathbf{u}_h \rangle_{0,\Omega} + \langle \varphi_i, (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_j \rangle_{0,\Omega} - \langle \Delta \varphi_i, \nu^2 \tau_m \Delta \varphi_j \rangle_{0,\Omega} - \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \nu \tau_m \Delta \varphi_j \rangle_{0,\Omega} + \langle \Delta \varphi_i, \nu \tau_m (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_j \rangle_{0,\Omega} + \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_j \rangle_{0,\Omega} + \langle \nabla \cdot \varphi_i, \tau_c \nabla \cdot \varphi_j \rangle_{0,\Omega}, \quad (19a)$$

$$C_{ij}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) = \frac{\partial \bar{R}_i(\hat{\mathbf{u}}, \hat{\mathbf{p}})}{\partial \hat{p}_j} = \langle \varphi_i, \nabla \varphi_j \rangle_{0,\Omega} + \langle \Delta \varphi_i, \nu \tau_m \nabla \varphi_j \rangle_{0,\Omega} + \langle (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_i, \tau_m \nabla \varphi_j \rangle_{0,\Omega}, \quad (19b)$$

$$\mathfrak{C}_{ij}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) = \frac{\partial \bar{R}_i(\hat{\mathbf{u}}, \hat{\mathbf{p}})}{\partial \hat{u}_j} = - \langle \varphi_i, \nabla \cdot \varphi_j \rangle_{0,\Omega} - \langle \nabla \varphi_i, \nu \tau_m \Delta \varphi_j \rangle_{0,\Omega} + \langle \nabla \varphi_i, \tau_m (\mathbf{u}_h - \mathbf{u}_d) \cdot \nabla \varphi_j \rangle_{0,\Omega}, \quad (19c)$$

$$\mathcal{K}_{ij}(\hat{\mathbf{u}}, \hat{\mathbf{p}}) = \frac{\partial \bar{R}_i(\hat{\mathbf{u}}, \hat{\mathbf{p}})}{\partial \hat{p}_j} = \langle \nabla \varphi_i, \tau_m \nabla \varphi_j \rangle_{0,\Omega}. \quad (19d)$$

Unconditional stability for the Bossak time integration algorithm can be ensured by choosing  $\gamma_b = 1/2 - \alpha_b$ . In the case of isogeometric finite elements where virtually all derivatives defined in Eqs. (14) are available, the following choice of the stabilization parameters is made [BMCH10],

$$\tau_m = \left( C_t dt^{-2} + \frac{\partial X_\alpha}{\partial \theta_\beta} u_{h,\alpha} u_{h,\beta} + C_i \nu^2 \frac{\partial X_\alpha}{\partial \theta_\beta} \frac{\partial X_\alpha}{\partial \theta_\beta} \right)^{-\frac{1}{2}}, \quad (20a)$$

$$\tau_c = \left( \tau_m \left\| \sum_{\alpha=1}^2 \frac{\partial \mathbf{X}}{\partial \theta_\alpha} \right\|_2^2 \right)^{-1}, \quad (20b)$$

where  $C_t = C_i = 4$  are empirical constants,  $\|\bullet\|$  is the Frobenious norm of a matrix,  $[\partial X_\alpha / \partial \theta_\beta]$  is the Jacobian matrix of the geometric transformation to the element's parametric space  $\theta_1$ - $\theta_2$ ,  $\partial \mathbf{X} / \partial \theta_\alpha$  is the base vector along the  $\theta_\alpha$ -parametric direction and  $\|\bullet\|_2$  stands for the 2-norm of a vector. On the other hand, in the case of linear finite elements, such as the *Constant Strain Triangle* (CST), where higher than first order derivatives in Eqs. (14) the stabilization parameters are chosen as [Cod01],

$$\tau_m = (C_t dt^{-1} + 2 h^{-1} \|\mathbf{u}_h\|_2 + C_i \nu h^{-2})^{-1}, \quad (21a)$$

$$\tau_c = (\nu + 0.5 h \|\mathbf{u}_h\|_2)^{-1}, \quad (21b)$$

where  $\mathbf{u}_h$  stands for the numerical velocity field at the integration point from the previous quasi-Newton iteration.

## 4 Steady-state formulation

For the steady-state formulation of the incompressible Navier-Stokes Eqs. (2) using the VMS stabilization method and the corresponding finite element discretization, the inertial terms are neglected. In this way, the  $\hat{i}$ -th quasi-Newton iteration becomes,

$$\begin{bmatrix} \mathbf{K}(\hat{\mathbf{u}}_i, \hat{\mathbf{p}}_i) & \mathcal{C}(\hat{\mathbf{u}}_i, \hat{\mathbf{p}}_i) \\ \mathcal{C}(\hat{\mathbf{u}}_i, \hat{\mathbf{p}}_i) & \mathcal{K}(\hat{\mathbf{u}}_i, \hat{\mathbf{p}}_i) \end{bmatrix} \begin{bmatrix} \Delta_i \hat{\mathbf{u}} \\ \Delta_i \hat{\mathbf{p}} \end{bmatrix} = - \begin{bmatrix} \bar{\mathbf{R}}(\hat{\mathbf{u}}_i, \hat{\mathbf{p}}_i) - \hat{\mathbf{F}}(\hat{\mathbf{u}}_i) \\ \bar{\mathcal{R}}(\hat{\mathbf{u}}_i, \hat{\mathbf{p}}_i) - \hat{\mathcal{F}} \end{bmatrix}. \quad (22)$$

Regarding the estimation of the stabilization parameters, the same formulas as in Eqs. (20) and (21) for the isogeometric and the low-order finite elements, respectively, hold also for the steady-state case with the only difference that  $C_t = 0$ .

Equation systems in Eqs. (18) and (22) are obviously unsymmetric and not necessarily well-conditioned. Preconditioners have been studied in the literature, see for example in [BMCH10], but in this work no preconditioners are used and the linear equation systems are solved as presented herein in 2D.

## 5 Steady-state drag optimization using finite differencing

Given is a portion of the domain's boundary  $\gamma_D \subset \Gamma$  over which the drag force  $f_D$  is sought. If  $\gamma_{D,h}$  stands for the geometric discretization of  $\gamma_D$  due to the finite element approximation of the primal fields, then

$$f_D(\mathbf{u}, p) = \frac{1}{\rho} \sum_{i \in \mathcal{I}_D} \bar{R}_{2i-1}(\hat{\mathbf{u}}, \hat{\mathbf{p}}), \quad (23)$$

where  $\mathcal{I}_D$  stands for the set of indices corresponding to the finite element nodes on  $\gamma_{D,h}$ . Eq. (23) is nothing else but the sum of all forces by means of the momentum residuals in Eq. (14c) acting on  $\gamma_{D,h}$  along the  $X_1$ -Cartesian direction depending on the unknown fields  $\mathbf{u}$  and  $p$ , which are in turn defined by their nodal values  $\hat{\mathbf{u}}$  and  $\hat{\mathbf{p}}$  within the finite element approximation in Eqs. (9).

Herein the unconstrained shape optimization of a cylinder in flow is considered. The only design variable is the radius of the cylinder  $r$  and the objective/cost function  $J(\mathbf{u}(r), p(r), r) = f_D(\mathbf{u}(r), p(r), r)$  is the drag force. It is expected that the cylinder collapses into a point since no other constraint is assumed. The optimization problem can then be formulated as follows,

$$r = \arg \min_{r'} J(\mathbf{u}(r'), p(r'), r') \quad (24a)$$

$$\text{s.t.} \quad \begin{bmatrix} \bar{\mathbf{R}}(\mathbf{u}(r), p(r)) \\ \bar{\mathcal{R}}(\mathbf{u}(r), p(r)) \end{bmatrix} = \mathbf{0} \text{ in } \Omega(r). \quad (24b)$$

Eqs. (24) demonstrate that there is an implicit dependence of the state to the design variable, that is,  $\mathbf{u} = \mathbf{u}(r)$  and  $p = p(r)$ . Within the Finite Differencing (FD) approach, problem in Eq. (24) is solved in a staggered iterative manner, see also in [Ble14]. Accordingly, at each optimization iteration/design update, the state variables  $\mathbf{u}$  and  $p$  are computed such that Eq. (24b) is satisfied, see Sec. 4. To minimize objective/cost function in Eq. (24a), its total variation should be equal to zero, that is,  $\delta f_D(\mathbf{u}(r), p(r)) = 0$ , which results in the following residual form,

$$s(\mathbf{u}(r), p(r), r) = \frac{\partial J}{\partial u_\alpha} \frac{\partial u_\alpha}{\partial r} + \frac{\partial J}{\partial p} \frac{\partial p}{\partial r} + \frac{\partial J}{\partial r}, \quad (25)$$

where  $\mathbf{u} = u_\alpha \mathbf{e}_\alpha$ . Eq. (25) is known as the sensitivity equation and is to be solved for the design update. Linearization of Eq. (25) results in,

$$H(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}}) \Delta_{\tilde{i}} r = -s(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}}) , \quad (26)$$

where  $\Delta_{\tilde{i}} r = r_{\tilde{i}+1} - r_{\tilde{i}}$  and  $\tilde{i}$  stands for the index of the optimization iteration. Hessian matrix  $H$  is given by,

$$H(\mathbf{u}(r), p(r), r) = \frac{\partial s(\mathbf{u}(r), p(r), r)}{\partial r} . \quad (27)$$

Herein, the Hessian matrix in Eq. (27) is approximated with the identity matrix, also because its computation is very costly. Therefore Eq. (26) becomes,

$$r_{\tilde{i}+1} = r_{\tilde{i}} - s(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}}) , \quad (28)$$

which indicates the the shape update must be in the direction opposite to the sensitivity. Another direct implication of choosing the identity matrix in the place of the Hessian is that no quadratic convergence in the neighborhood of the solution must be expected. The Hessian on the other hand might be ill-conditioned dependent on the primal problem, the design variables and the objection function which often requires the use of preconditioners.

As aforementioned, for each design update  $r_{\tilde{i}}$  the primal variables  $\mathbf{u}(r_{\tilde{i}})$  and  $p(r_{\tilde{i}})$  are updated such that Eq. (24b) is satisfied. Then, within FD given a small enough perturbation parameter  $\epsilon_{\tilde{i}} > 0$ , sensitivity  $s(\mathbf{u}_{\tilde{i}}(r_{\tilde{i}}), p_{\tilde{i}}(r_{\tilde{i}}), r_{\tilde{i}})$  in Eq. (25) is computed as,

$$s(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}}) \approx \frac{J(\mathbf{u}(r_{\tilde{i}} + \epsilon), p(r_{\tilde{i}} + \epsilon), r_{\tilde{i}} + \epsilon) - J(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}})}{\epsilon} . \quad (29)$$

1. Initialize optimization counter  $\tilde{i} = 1$  and design parameter  $r_1 = r_0$ ;

**while**  $J(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}}) > \epsilon \wedge \tilde{i} \leq n_{\max}$  **do**

- 1i. Solve the primal problem in Eq. (22) for the design  $r_{\tilde{i}}$  to obtain objective  $J(\mathbf{u}(r_{\tilde{i}}), p(r_{\tilde{i}}), r_{\tilde{i}})$ ;
- 1ii. Evaluate convergence conditions and if they are fulfilled break the loop;
- 1iii. Solve the perturbed system in Eq. (22) for the design  $r_{\tilde{i}} + \epsilon$  to obtain objective  $J(\mathbf{u}(r_{\tilde{i}} + \epsilon), p(r_{\tilde{i}} + \epsilon), r_{\tilde{i}} + \epsilon)$ ;
- 1iv. Compute the sensitivity using Eq. (29);
- 1v. Update the design using Eq. (28) ;
- 1vi. Update the optimization iteration  $\tilde{i} + +$ ;

**end**

**Algorithm 1:** Unconstrained optimization using finite differencing

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