PhD Report
PDE-Constrained Shape Optimization in Fluid Dynamics

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Contents

Nomenclature

General notations

- $\mathbb{R}_{>0} \coloneqq (0, \infty)$, $\mathbb{R}_{\geq 0} \coloneqq [0, \infty)$, $\mathbb{R}_{<0} \coloneqq (-\infty, 0)$, $\mathbb{R}_{\leq 0} \coloneqq (-\infty, 0]$.
- δ_{ij}: Kronecker tensor, $\delta_{ij} = 1$ if $i = j$, $\delta_{ij} = 0$ if $i \neq j$.
- $\mathbf{u} = (u_1, \ldots, u_N) \in \mathbb{R}^N$: velocity vector field.[1]
- $p \in \mathbb{R}$: pressure scalar field.
- $\boldsymbol{\varepsilon}(\mathbf{u}) \coloneqq \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^\top)$: the *symmetrized gradient* of a vector field.
- $\mathbf{u} \otimes \mathbf{u} \coloneqq (u_i u_j)_{i,j=1}^N$, which is a 2nd-order tensor.
- $\mathrm{Re} \coloneqq \frac{UL}{\nu}$: Reynolds number.
- D: domain in $\mathbb{R}^d$ with piecewise smooth boundary ∂D
- Ω: measurable set in $\mathbb{R}^d$ or in D, or domain of class C^k
- $\partial\Omega$: boundary of Ω
- $\mathbf{n}$: unit outward normal vector field on Γ
- $\mathcal{N}_0$: unitary extension of $\mathbf{n}$ to an open neighborhood of Γ in $\mathbb{R}^d$
- χ_Ω: characteristic function of Ω
- $\Omega^c = D \backslash \overline{\Omega}$ (or $\mathbb{R}^d \backslash \overline{\Omega}$)
- $|\Omega|$: d-dimensional measure of Ω
- κ: mean curvature of Γ
- $P_D(\Omega)$: perimeter of Ω in D
- T_t: transformation of $\mathbb{R}^d$ or of $\overline{D}$ into $\mathbb{R}^d$
- DT_t: Jacobian of T_t
- $dJ[V](\Omega)$: Eulerian derivative

[1] In the literature of fluid dynamics, it is common to denote by $\mathbf{v}$ the velocity vector field. But in this thesis, the author has to deal primarily with adjoint methods, so $\mathbf{v}$ is used to denote the *adjoint velocity vector field* instead.

- γ_Γ: trace operator on Γ, e.g. $\gamma_\Gamma \in \mathcal{L}(H^1(\Omega); H^{1/2}(\Gamma))$
- ∇_Γ: tangential gradient on Γ
- $\partial_{\mathbf{n}}$: normal derivative on Γ
- div_Γ: tangential divergence on Γ
- Δ_Γ: Laplace-Beltrami operator on Γ
- $du[V](\Omega)$: material derivative of $u(\Omega)$ at Ω in the direction of the vector field V
- $u'[V](\Omega)$: local shape derivative of $u(\Omega)$ at Ω in the direction of the vector field V

Notations for matrix-vector operations

Given $N \in \mathbb{Z}_{\geq 0}$, let $\mathbf{x} = (x_i)_{i=1}^N$ and $\mathbf{y} = (y_i)_{i=1}^N$ be two column vectors and $A = (a_{ij})_{i,j=1}^N$ and $B = (b_{ij})_{i,j=1}^N$ be two $N \times N$ matrices.

- $\mathbf{x}^\top$, $A^\top$: transpose vector and transpose matrix of $\mathbf{x}$ and A, respectively.
- The *dot product/scalar product/inner product* of 2 vectors is

$$\mathbf{x} \cdot \mathbf{y} \coloneqq \sum_{i=1}^N x_i y_i.$$

- The *dyalic product* of 2 vectors of length N is a $N \times N$ matrix:

$$\mathbf{x} \otimes \mathbf{y} \equiv \mathbf{x}\mathbf{y}^\top \coloneqq (x_i y_j)_{i,j=1}^N.$$

- Bilinear form:

$$\mathbf{x}^\top A \mathbf{y} \coloneqq \sum_{i=1}^N \sum_{j=1}^N x_i a_{ij} y_j, \ \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^N.$$

- The *dot product* of 2 matrices is a scalar

$$A : B \coloneqq \sum_{i,j=1}^N a_{ij} b_{ij}.$$

- For any $\phi : \mathbb{R}^N \to \mathbb{R}$, define

$$\partial_{\mathbf{n}} \phi \coloneqq \nabla \phi \cdot \mathbf{n} = \mathbf{n} \cdot \nabla \phi = \sum_{i=1}^N n_i \partial_{x_i} \phi.$$

- For any vector field $\boldsymbol{\phi} : \mathbb{R}^N \to \mathbb{R}^N$, define

$$\mathrm{div}\, \boldsymbol{\phi} \coloneqq \nabla \cdot \boldsymbol{\phi} \coloneqq \sum_{i=1}^N \partial_{x_i} \phi_i,$$

$$\nabla\boldsymbol{\phi} \coloneqq (\partial_{x_i}\phi_j)_{i,j=1}^N,\ \mathrm{D}\boldsymbol{\phi} \coloneqq (\nabla\boldsymbol{\phi})^\top = (\partial_{x_j}\phi_i)_{i,j=1}^N,$$

$$\boldsymbol{\phi}\cdot\nabla\boldsymbol{\phi} \coloneqq (\boldsymbol{\phi}\cdot\nabla)\boldsymbol{\phi} \coloneqq \left(\sum_{j=1}^N \phi_j\partial_{x_j}\phi_i\right)_{i=1}^N \in \mathbb{R}^N,$$

$$\partial_{\mathbf{n}}\boldsymbol{\phi} \coloneqq \mathbf{n}\cdot\nabla\boldsymbol{\phi} = \mathrm{D}\boldsymbol{\phi}\cdot\mathbf{n} = \left(\sum_{i=1}^N n_i\partial_{x_i}\phi_j\right)_{j=1}^N \in \mathbb{R}^N,$$

$$\boldsymbol{\varepsilon}_{\mathbf{n}}(\boldsymbol{\phi}) \coloneqq \boldsymbol{\varepsilon}(\boldsymbol{\phi})\cdot\mathbf{n} = \boldsymbol{\varepsilon}(\boldsymbol{\phi})\mathbf{n} = \left(\sum_{i=1}^N n_i\varepsilon_{ij}(\boldsymbol{\phi})\right)_{j=1}^N = \left(\sum_{i=1}^N \frac{1}{2}n_i(\partial_{x_i}\phi_j + \partial_{x_j}\phi_i)\right)_{j=1}^N \in \mathbb{R}^N.$$

Remark 0.0.1 (Convention)**.** *For clarity instead of brevity, we do not use Einstein summation convention and Levi-Civita tensor, which is fully characterized by $\varepsilon_{123} = 1$ and ε_{ijk} is antisymmetric against the indices.*

Remark 0.0.2 (Notation)**.** *In general, scalar quantities are denoted by small letters, vectors and vector-valued functions will be denoted in bold small letters, and matrices or tensors by capital letters, e.g.* $\mathbf{u}(t,\mathbf{x})$, $p(t,\mathbf{x})$.

Remark 0.0.3 (Bilinear form)**.** *For any $A \in \mathrm{Mat}_N(\mathbb{R})$, the bilinear form*

$$\begin{aligned} B_A : \mathbb{R}^N \times \mathbb{R}^N &\to \mathbb{R} \\ (\mathbf{x},\mathbf{y}) &\mapsto B_A(\mathbf{x},\mathbf{y}) \coloneqq \mathbf{x}^\top A\mathbf{y} = \sum_{i=1}^N\sum_{j=1}^N x_i a_{ij} y_j, \end{aligned}$$

can be rewritten in other representations as follows:

$$B_A(\mathbf{x},\mathbf{y}) = \mathbf{x}^\top A\mathbf{y} = (A\mathbf{y})\cdot\mathbf{x} = (A^\top\mathbf{x})^\top\mathbf{y} = (A^\top\mathbf{x})\cdot\mathbf{y} = (\mathbf{x}\otimes\mathbf{y}) : A = (\mathbf{x}\mathbf{y}^\top) : A.$$

As a consequence, when $A = \nabla\mathbf{u}$ for some vector $\mathbf{u}$, one has

$$\mathbf{n}^\top\nabla\mathbf{u}\mathbf{v} = ((\nabla\mathbf{u})^\top\mathbf{n})\cdot\mathbf{v} = (\mathrm{D}\mathbf{u}\mathbf{n})\cdot\mathbf{v} = \partial_{\mathbf{n}}\mathbf{u}\cdot\mathbf{v}.$$

Acronyms

1. 1D/2D/3D: one-/two-/three-dimensional
2. a.e.: almost everywhere
3. a.a.: almost all
4. BVP(s): boundary value problem(s)
5. CFD: Computational Fluid Dynamics
6. DNS: Direct Numerical Simulation
7. e.g.: for example, for instance
8. FD(M)(s): finite difference (method)(s)
9. FE(M)(s): finite element (method)(s)
10. FV(M)(s): finite volume (method)(s)
11. LES: Large Eddy Simulation
12. OSD(s): optimal shape design(s)
13. ODE(s): ordinary differential equation(s)
14. PDE(s): partial differential equation(s)
15. SOP(s): shape optimization problem(s)
16. s.t.: such that
17. w.r.t.: with respect to

Chapter 1

Introductions

1.1 Short introduction to PDEs

1.1.1 Nonhomogeneous BVPs

Let Ω be an open subset of $\mathbb{R}^N$, $N \in \mathbb{Z}_{\geq 0}$, with boundary $\Gamma \coloneqq \partial\Omega$. In Ω and on Γ, we introduce, respectively, *differential operators* P and Q_i, $0 \leq i \leq n_{\mathrm{bc}}$, where n_{bc} is the number of boundary conditions.

In Lions and Magenes, 1972, the authors defined the concept of *nonhomogeneous boundary value problem* as a problem of the following type: let f and g_i, $0 \leq i \leq n_{\mathrm{bc}}$, be given in function spaces F and G_i, $0 \leq i \leq n_{\mathrm{bc}}$, respectively, where F is a space defined "on Ω and the G_i's spaces are defined "on Γ; we seek u in a function space $\mathcal{U}$ "on Ω" satisfying

$$\begin{cases} Pu = f, & \text{in } \Omega, \\ Q_i u = g_i, & \text{on } \Gamma,\ \forall i = 1, \ldots, n_{\mathrm{bc}}. \end{cases} \tag{gnhBVP}$$

The Q_i's are called *boundary operators* to distinguish these and the (domain) operator P.

Note that it can happen, which is the case of most evolutionary problems, that $Q_i \equiv 0$ on some part of Γ, so that the number n_{bc} of boundary conditions may depend on the part of Γ considered.

1.1.1.1 Weak formulations of nonhomogeneous BVPs

Multiply both side of the first equation in (gnhBVP) with v and then integrate by parts all the high-order terms to obtain the weak formulation of (gnhBVP).

In the study of weak formulations, we recall the theorems of Stampacchia and Lax–Milgram (see, e.g., Brezis, 2011, Sect. 5.3, Temam, 2000, Subsect. I.2.2).

Definition 1.1.1 (Continuous/coercive bilinear form). *A bilinear form $a : H \times H \to \mathbb{R}$ is said to be*

(i) continuous *if there is a constant C such that*

$$|a(u, v)| \leq C\|u\|_H\|v\|_H,\ \forall u, v \in H;$$

(ii) coercive *if there is a constant $\alpha > 0$ such that*

$$a(v, v) \geq \alpha\|v\|_H^2,\ \forall v \in H.$$

Theorem 1.1.1 (Stampacchia)**.** *Assume that $a(u, v)$ is a continuous coercive bilinear form on H. Let $K \subset H$ be a nonempty closed and convex subset. Then, given any $\phi \in H^\star$, there exists a unique element $u \in K$ such that*

$$a(u, v-u) \geq \langle \phi, v-u \rangle_{H^\star, H}, \ \forall v \in K.$$

Moreover, if a is symmetric, then u is characterized by the property

$$u \in K, \ \frac{1}{2}a(u,u) - \langle \phi, u \rangle_{H^\star, H} = \min_{v \in K} \frac{1}{2}a(v,v) - \langle \phi, v \rangle_{H^\star, H}.$$

Proof. See, e.g., Brezis, 2011, pp. 138–140. □

Applying Theorem 1.1.1 with $K = H$ yields the following corollary.

Theorem 1.1.2 (Lax-Milgram)**.** *Assume that $a(u, v)$ is a continuous coercive bilinear form on H. Then, given any $\phi \in H^\star$, there exists a unique element $u \in H$ such that*

$$a(u, v) = \langle \phi, v \rangle_{H^\star, H}, \ \forall v \in H. \tag{1.1.1}$$

Moreover, if a is symmetric, then u is characterized by the property

$$u \in H, \ \frac{1}{2}a(u,u) - \langle \phi, u \rangle_{H^\star, H} = \min_{v \in H} \frac{1}{2}a(v,v) - \langle \phi, v \rangle_{H^\star, H}. \tag{1.1.2}$$

Remark 1.1.1. *In the language of the* calculus of variations*, (1.1.1) is the* Euler equation $F'(u) = 0$ *associated with the minimization problem (1.1.2) with $F(v) \coloneqq \frac{1}{2}a(v,v) - \langle \phi, v \rangle$.*

1.1.1.2 Unbounded linear operators and adjoint

We recall the following definitions from Brezis, 2011, Sect. 2.6.

Definition 1.1.2 (Unbounded linear operator)**.** *Let E and F be two Banach spaces. An* unbounded linear operator *from E into F is a linear map $A : D(A) \subset E \to F$ defined on a linear subspace $D(A) \subset E$ with values in F. The set $D(A)$ is called the* domain *of A.*

One says that A is bounded *(or* continuous*) if $D(A) = E$ and if there is a constant $c \geq 0$ such that*

$$\|Au\| \leq c\|u\|, \ \forall u \in E.$$

The norm of a bounded operator is defined by

$$\|A\|_{\mathcal{L}(E,F)} \coloneqq \sup_{u \neq 0} \frac{\|Au\|}{\|u\|}.$$

Definition 1.1.3 (Adjoint)**.** *Let $A : D(A) \subset E \to F$ be an unbounded linear operator that is* densely defined*. We define an unbounded operator $A^\star : D(A^\star) \subset F^\star \to E^\star$ as follows. One defines its domain:*

$$D(A^\star) \coloneqq \{v \in F^\star; \exists c \geq 0 \text{ such that } |\langle v, Au \rangle| \leq c\|u\|, \ \forall u \in D(A)\},$$

which is clearly is a linear subspace of $F^\star$. Given $v \in D(A^\star)$, consider the map $g : D(A) \to \mathbb{R}$ defined by

$$g(u) = \langle v, Au \rangle, \ \forall u \in D(A).$$

Since $|g(u)| \le c\|u\|$, $\forall u \in D(A)$, applying Hahn–Banach theorem yields that there exists a linear map $f : E \to \mathbb{R}$ that extends g and s.t. $|f(u)| \le c\|u\|$, $\forall u \in E$, and thus $f \in E^\star$. Note that the extension of g is unique, since $D(A)$ is dense in E. Set $A^\star v = f$.

The unbounded linear operator $A^\star : D(A^\star) \subset F^\star \to E^\star$ is called the adjoint *of A. Briefly, the fundamental relation between A and $A^\star$ is given by*

$$\langle v, Au\rangle_{F^\star,F} = \langle A^\star v, u\rangle_{E^\star,E}, \ \forall u \in D(A), \ \forall v \in D(A^\star).$$

1.1.2 Abstract linear saddle point problems*

See John, 2016, Chap. 3.

1.2 Introduction to Shape Optimization

$$\min_{\Omega\in\mathcal{O}_{\rm ad}} J(U,\Omega) \text{ s.t. } E(U,\Omega) = 0. \tag{sop}$$

1.2.1 Cost/Objective functionals

The problem of how to choose appropriate cost/objective functional to quantify the control objective is an important topic in the field of optimal control of PDEs. This functional, say J, depends on the *state variables* U and on the control parameters describing the shape of the domain, i.e., $J(U,\Omega)$.

- Tracking-type functionals:

$$J_{\rm trk}(\mathbf{u},\tilde{\Omega}) := \int_{\tilde{\Omega}} |\mathbf{u} - \mathbf{u}_{\rm d}|^2 {\rm d}\mathbf{x}, \text{ for some } \tilde{\Omega} \subset \Omega, \tag{trk-func}$$

  where $\mathbf{u}_{\rm d} : \Omega \to \mathbb{R}^N$ is a given desired flow field which contains some expected features of the controlled flow field.

- Minimization of curl of the velocity field:

$$J_{\rm curl}(\mathbf{u},\tilde{\Omega}) := \frac{1}{2}\int_{\tilde{\Omega}} |\nabla \times \mathbf{u}|^2 {\rm d}\mathbf{x}, \text{ for some } \tilde{\Omega} \subset \Omega. \tag{curl-func}$$

- See Hintermüller et al., 2004, A Galilean invariant cost functional:

$$J(\mathbf{u},\tilde{\Omega}) := \int_{\tilde{\Omega}} \max\{0, \det \nabla\mathbf{u}\} {\rm d}\mathbf{x}, \text{ for some } \tilde{\Omega} \subset \Omega.$$

  In Kasumba, 2010, the following smoothed cost functional is introduced to treat the non-differentiability of the previous cost functional due to the max operation:

$$J(\mathbf{u},\tilde{\Omega}) := \int_{\tilde{\Omega}} g(\det \nabla\mathbf{u}) {\rm d}\mathbf{x}, \text{ with } g(t) := \begin{cases} 0, & t \le 0, \\ \dfrac{t^3}{1+t^2}, & t > 0. \end{cases}$$

  Note that alternatives for the smoothing function g can be chosen.

- In Kasumba, 2010, the author considered the following generalized cost functional:

$$J(u,\Omega) \coloneqq \int_\Omega j(C_\gamma u),\ \text{where } C_\gamma : u \mapsto Cu+\gamma,\ \gamma \in L^2(\Omega),$$

  Note that C_γ is an *affine operator*.

- In Ito, Kunisch, and Peichl, 2006, the authors consider

$$J(u,\Gamma) \coloneqq \frac{1}{2}\int_\Gamma u^2 \mathrm{d}\Gamma,$$

  where $u = u(\Gamma)$ is a solution of the mixed BVP

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = g_d, & \text{on } \Gamma_d, \\ \partial_{\mathbf{n}} u = g, & \text{on } \Gamma. \end{cases}$$

In this thesis, we consider the following general cost functional:

$$J(\mathbf{u},p,\Omega) \coloneqq \int_\Omega J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x} + \int_\Gamma J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathrm{d}\Gamma. \tag{cost-func-NS}$$

To calculate the shape derivative of this cost functional, we consider the its perturbed analogue:

$$J(\mathbf{u}_t,p_t,\Omega_t) \coloneqq \int_{\Omega_t} J_\Omega(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t)\mathrm{d}\mathbf{x} + \int_{\Gamma_t} J_\Gamma(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t,\mathbf{n}_t,\mathbf{t}_t)\mathrm{d}\Gamma_t, \tag{ptb-cost-func-NS}$$

where $(\mathbf{u}_t, p_t)$ denotes the strong/classical solution of (gS) on the perturbed domain $\Omega_t \coloneqq T_t(V)(\Omega)$.

1.2.2 Shape sensitivities

1.3 Sensitivity analysis in shape optimization

We use the material derivative approach. The following presentation will be formal, i.e. it is correct provided that all necessary variables are sufficiently smooth. Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with Lipschitz boundary $\Gamma \coloneqq \partial\Omega$. We introduce a one-parameter family of mappings $\{T_t\}$, $t \in [0,t_0]$, $T_t : \Omega \to \mathbb{R}^d$ such that $T_0 = \mathrm{id}$, where id is the identity mapping of $\mathbb{R}^d$. Denote

$$x_t \coloneqq T_t(x),\ x \in \Omega,\ t \in [0,t_0]. \tag{1.3.1}$$

The perturbed domain at time t is given by $\Omega_t \coloneqq T_t(\Omega)$, $t \in [0,t_0]$. We assume additionally that each T_t, $t \in [0,t_0]$, has to be a one-to-one transformation of Ω onto Ω_t such that

$$T_t(\operatorname{int}\Omega) = \operatorname{int}\Omega_t,\ T_t(\partial\Omega) = \partial\Omega_t. \tag{1.3.2}$$

Denote also $\Gamma_t \coloneqq \partial\Omega_t$. In the remaining of this text, we consider $\{T_t\}_t$ as a perturbation of the identity, i.e.

$$T_t[V] \coloneqq \mathrm{id} + tV,\ t > 0, \tag{1.3.3}$$

where $V \in W^{1,\infty}(\Omega)^d$ is the so-called *velocity field*.

Lemma 1.3.1. *For t_0 small enough, T_t of the form (1.3.3) is a one-to-one mapping of Ω onto Ω_t satisfying (1.3.2) and preserving the Lipschitz continuity of $\partial\Omega_t$.*

The shape derivative of J at Ω in the direction of the deformation field V is defined as the limit

$$dJ(\Omega)V = \lim_{t\to 0} \frac{J(\Omega_t) - J(\Omega)}{t}, \tag{1.3.4}$$

provided that it exists. If the mapping $V \mapsto dJ(\Omega)V$ is linear and continuous, then we say that $J(\Omega)$ is *shape differentiable.*

Let DT_t denote the Jacobian of T_t. The following lemma lists some formula concerning their differentiation.

Lemma 1.3.2. *The following formulas hold:*

(i) $DT_t|_{t=0} = \mathrm{id}$.

(ii) $\frac{d}{dt}T_t\big|_{t=0} = V$.

(iii) $\frac{d}{dt}DT_t\big|_{t=0} = DV$.

(iv) $\frac{d}{dt}(DT_t)^\top\big|_{t=0} = DV^\top$.

(v) $\frac{d}{dt}DT_t^{-1}\big|_{t=0} = -DV$.

(vi) $\frac{d}{dt}\det DT_t\big|_{t=0} = \nabla\cdot V$.

We consider a state problem, say (P) in a domain $\Omega \subset \mathbb{R}^d$. Let (P_t), $t \in (0, t_0]$, be a family of problems related to (P) but solved in Ω_t with T_t given by (1.3.3). Solution of (P_t) will be denoted by u_t defined on Ω_t.

Definition 1.3.1 (Material derivative, local derivative)**.** *Let u_t solve (P_t) on the perturbed domain $\Omega_t := T_t[V](\Omega)$ and let $x_t := T_t[V](x)$ be the shifted point of a point $x \in \Omega$. Then material derivative is defined by*

$$du[V](x) := \frac{d}{dt}\bigg|_{t=0} u_t(x_t), \tag{1.3.5}$$

and the local shape derivative *is defined by*

$$u'[V](x) := \frac{d}{dt}\bigg|_{t=0} u_t(x). \tag{1.3.6}$$

Lemma 1.3.3. *The chain rule allows the material and local shape derivatives to be converted into each other:*

$$du[V] = u'[V] + \nabla u \cdot V. \tag{1.3.7}$$

Theorem 1.3.1 (Hadamard)**.** *For $f \in C(\overline{\Omega})$ the directional shape derivative of the domain integral $\int_\Omega f(x)\mathrm{d}x$ is the boundary integral*

$$d\left(\int_\Omega f(x)\mathrm{d}x\right)[V] = \int_\Gamma \langle V, \mathbf{n}\rangle f(x)\mathrm{d}s. \tag{1.3.8}$$

1.4 Shape calculus

Consider the following shape functional, with $f \in L^2(D)$, $j : D \times \mathbb{R} \to \mathbb{R}$:

$$J(\Omega) := \int_\Omega j(x, u(x))\mathrm{d}x, \tag{1.4.1}$$

where $u : \Omega \to \mathbb{R}$ satisfies (1.5.1).

We now want to calculate the shape derivative of (1.4.1). For this purpose, consider the *perturbed cost functional*

$$J(\Omega_t) := \int_{\Omega_t} j(x_t, u_t(x_t))\mathrm{d}x_t, \tag{1.4.2}$$

where u_t denotes the weak solution of (1.5.1) on the domain $\Omega_t[V]$, i.e., $u_t \in H_0^1(\Omega_t[V])$ solves

$$(\nabla u_t, \nabla v)_{L^2(\Omega_t[V])} = (f, v)_{L^2(\Omega_t[V])}, \ \forall v \in H_0^1(\Omega_t[V]). \tag{1.4.3}$$

By Theorem 1.5.1, there exists a unique weak solution $u_t \in H_0^1(\Omega_t[V])$ of the perturbed BVP:

$$\begin{cases} -\Delta u_t = f & \text{in } \Omega_t, \\ u_t = 0 & \text{on } \Gamma_t, \end{cases} \tag{1.4.4}$$

which satisfies

$$\|u_t\|_{H_0^1(\Omega_t[V])} \leq C\|f\|_{L^2(\Omega_t[V])}. \tag{1.4.5}$$

By Theorem 1.5.2, with the assumption that Ω_t has C^2-boundary, in particular we assume $\partial\Omega$ is C^2 and $V \in C^2(\overline{D}, \mathbb{R}^d)$, the weak solution $u_t \in H_0^1(\Omega_t[V])$ of the problem (1.4.4) satisfies $u_t \in H^2(\Omega_t[V])$ and

$$\|u_t\|_{H^2(\Omega_t[V])} \leq C\|f\|_{L^2(\Omega_t[V])}. \tag{1.4.6}$$

By Lemma 1.3.3, this yields

$$dJ(\Omega)[V] = \int_\Gamma \langle V, \mathbf{n}\rangle j(x, g)\mathrm{d}s + \int_\Omega \frac{\partial j}{\partial u}(x, u)du[V]\mathrm{d}x. \tag{1.4.7}$$

We have

$$\begin{cases} \Delta u'[V] = 0 & \text{in } \Omega, \\ u'[V] = -\langle V, \mathbf{n}\rangle \partial_\mathbf{n} u & \text{on } \Gamma. \end{cases}$$

The 1st equation is deduced from

$$\Delta u'(x)[V] = \lim_{t\to 0} \frac{\Delta u_t[V](x) - \Delta u(x)}{t} = 0, \tag{1.4.8}$$

since both $u_t[V]$ and u satisfy Poisson equation.

For the 2nd boundary condition, apply the following lemma:

Lemma 1.4.1. *Let u satisfy*

$$u = u_b \text{ on } \partial\Omega, \tag{1.4.9}$$

where u_b does not depend on the geometry of Ω, i.e., independent of e.g. the outer normal.
The local shape derivative under a displacement field V is then given by the solution of

$$u'[V] = \langle V, \mathbf{n}\rangle \partial_{\mathbf{n}}(u_b - u) \text{ on } \Gamma, \tag{1.4.10}$$
$$u'[V] = 0 \text{ on } \partial\Omega\backslash\Gamma \tag{1.4.11}$$

where Γ here is only the variable part of the boundary $\partial\Omega$.

Proof. If the material derivative is taken from both sides of the Dirichlet boundary condition, you get

$$du[V] = du_b[V] \text{ on } \Gamma. \tag{1.4.12}$$

By

$$u'[V] + \langle \nabla u, V\rangle = du[V] = du_b[V] = \langle \nabla u_b, V\rangle, \tag{1.4.13}$$

since u_b does not depend on the geometry and thus $u_b'[V] = 0$. Thus $u'[V] = \langle \nabla(u_b - u), V\rangle$. Plugging in $\widetilde{V} := \langle V, \mathbf{n}\rangle\mathbf{n}$, we get

$$u'[V] = \langle V, \mathbf{n}\rangle \frac{\partial(u_b - u)}{\partial \mathbf{n}}, \tag{1.4.14}$$

which corresponds to the statement. □

Introduce the *adjoint state function* v according to

$$\begin{cases} -\Delta v = \dfrac{\partial j}{\partial u}(\cdot, u) & \text{in } \Omega, \\ \quad v = 0 & \text{on } \Gamma, \end{cases} \tag{1.4.15}$$

apply Green's 2nd formula

$$dJ(\Omega)[V] = \int_\Gamma \langle V, \mathbf{n}\rangle j(x,g)\mathrm{d}s - \int_\Omega v\Delta u'[V](x)\mathrm{d}x + \int_\Gamma \left(u'[V]\partial_{\mathbf{n}} v - v\frac{\partial u'[V]}{\partial \mathbf{n}}\right)\mathrm{d}s \tag{1.4.16}$$
$$= \int_\Gamma \langle V, \mathbf{n}\rangle j(x,g)\mathrm{d}s + \int_\Gamma u'[V]\partial_{\mathbf{n}} v \mathrm{d}s, \tag{1.4.17}$$

to derive the *boundary integral representation of the shape derivative*

$$dJ(\Omega)[V] = \int_\Gamma \langle V, \mathbf{n}\rangle \left(j(x,g) - \partial_{\mathbf{n}} u \partial_{\mathbf{n}} v\right)\mathrm{d}s. \tag{1.4.18}$$

Apply this formula for $j(x,g) = \frac{1}{2}(u(x) - z(x))^2$, we obtain

$$dJ(\Omega)[V] = \int_\Gamma \langle V, \mathbf{n}\rangle \left(\frac{1}{2}z^2 - \partial_{\mathbf{n}} u \partial_{\mathbf{n}} v\right)\mathrm{d}s. \tag{1.4.19}$$

Lemma 1.4.2 (Shape derivative formulas). *For τ_0 sufficiently small, $f \in C([0,\tau_0], W^{1,1}(D))$, and assume that $f_t(0)$ exists in $L^1(\Omega)$. Then*

$$\frac{d}{dt}\int_{\Omega_t} f(t,x_t)\mathrm{d}x_t|_{t=0} = \int_\Omega f_t(0,x)\mathrm{d}x + \int_\Gamma f(0,x)V\cdot\mathbf{n}\mathrm{d}s \tag{1.4.20}$$

Moreover, if $f \in C([0,\tau_0], W^{2,1}(\Omega))$, then

$$\frac{d}{dt}\int_{\Gamma_t} f(t,s_t)\mathrm{d}s_t|_{t=0} = \int_\Gamma f_t(0,s)ds + \int_\Gamma (\partial_{\mathbf{n}} f(0,s) + \kappa f(0,s))V\cdot\mathbf{n}\mathrm{d}s, \tag{1.4.21}$$

where κ stands for the mean curvature of Γ.

Definition 1.4.1 (Tangential divergence). *(i) Let Ω be a given domain with the boundary Γ of class C^2, and $V \in C^1(U;\mathbb{R}^d)$ be a vector field; U is an open neighborhood of the manifold $\Gamma \subset \mathbb{R}^d$. We define the* tangential divergence *of V as*

$$\mathrm{div}_\Gamma V = (\nabla\cdot V - \langle DV\cdot\mathbf{n},\mathbf{n}\rangle_{\mathbb{R}^d})|_\Gamma \in C(U). \tag{1.4.22}$$

(ii) Let Ω be a bounded domain with the boundary of class C^2, and let $V \in C^1(\Gamma;\mathbb{R}^d)$ be a given vector field on Γ. The tangential divergence *of V on Γ is given by*

$$\mathrm{div}_\Gamma V = (\mathrm{div}\widetilde{V} - \langle D\widetilde{V}\cdot\mathbf{n},\mathbf{n}\rangle_{\mathbb{R}^d})|_\Gamma \in C(\Gamma), \tag{1.4.23}$$

where $\widetilde{V}$ is any C^1 extension of V to an open neighborhood of $\Gamma \subset \mathbb{R}^d$.

See Sturm, 2015a; Sturm, 2015b for a survey of various methods used to compute shape sensitivities.

1. Rearrangement method, see Ito, Kunisch, and Peichl, 2008
2. An approach using a novel adjoint equation, see Sturm's WIAS preprint.
3. Material/shape derivative method, also called chain-rule approach, see Sokołowski and Jean-Paul Zolésio, 1992.
4. Min approach for energy cost functional, see Delfour, 2012.
5. Minimax approach, see Delfour and J.-P. Zolésio, 1988a.
6. Penalization method, see Delfour and J.-P. Zolésio, 1988b.
7. Céa's Lagrange method in Céa, 1986 is used to derive the formulas for the shape derivative, however, it does not prove the shape differentiability. See Pantz, 2005 for examples where Céa's method fails.

1.4.1 A min formulation for variational formulations

Let Ω be a bounded open domain in $\mathbb{R}^N$ with a smooth boundary Γ.

1.4.2 A min formulation for variational inequalities*

1.5 Shape Derivatives for Poisson Equation

1.5.1 Well-posedness of Poisson equation

We consider the Poisson equation

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma. \end{cases} \tag{1.5.1}$$

A function $y \in H_0^1(\Omega)$ is called a *weak solution* of (1.5.1) if it satisfies the *weak formulation*

$$(\nabla u, \nabla v)_{L^2(\Omega)} = (f, v)_{L^2(\Omega)}, \ \forall v \in H_0^1(\Omega). \tag{1.5.2}$$

Theorem 1.5.1 (Existence)**.** *Assume $f \in L^2(\Omega)$, then there exists a unique weak solution $u \in H_0^1(\Omega)$ of (1.5.1). Moreover, u satisfies*

$$\|u\|_{H_0^1(\Omega)} \leq C\|f\|_{L^2(\Omega)}, \tag{1.5.3}$$

where C is a constant depending only on Ω.

Proof. Define for u and v in $H_0^1(\Omega)$ the bilinear and linear forms

$$a(u, v) := (\nabla u, \nabla v)_{L^2(\Omega)}, \quad F(v) := (f, v)_{L^2(\Omega)},. \tag{1.5.4}$$

The boundedness and H_0^1-coercive of the bilinear form a follow directly. The form F is linear and $F \in (H_0^1(\Omega))^\star = H^{-1}(\Omega)$ due to Poincaré inequality:

$$|F(v)| \leq C\|f\|_{L^2(\Omega)}\|v\|_{H_0^1(\Omega)}, \ \forall v \in H_0^1(\Omega). \tag{1.5.5}$$

Using Lax-Milgram lemma, the variational equation (1.5.2) has a unique solution $u \in H_0^1(\Omega)$ which satisfies

$$\|u\|_{H_0^1(\Omega)} \leq \|F\|_{H^{-1}(\Omega)} \leq C\|f\|_{L^2(\Omega)}. \tag{1.5.6}$$

□

Theorem 1.5.2 (Higher regularity)**.** *Let $\Omega \subset \mathbb{R}^d$ be open, bounded with C^2-boundary. Then for any $f \in L^2(\Omega)$, the weak solution $u \in H_0^1(\Omega)$ of (1.5.1) satisfies $u \in H^2(\Omega)$ and*

$$\|u\|_{H^2(\Omega)} \leq C\|f\|_{L^2(\Omega)}, \tag{1.5.7}$$

with $C > 0$ depending only on Ω.

Proof. By Alt, 2016,

$$\|u\|_{H^2(\Omega)} \leq C\left(\|u\|_{H^1(\Omega)} + \|f\|_{L^2(\Omega)}\right). \tag{1.5.8}$$

Applying the estimate from the previous theorem, we get

$$\|u\|_{H^2(\Omega)} \leq C\left(\|u\|_{H_0^1(\Omega)} + \|f\|_{L^2(\Omega)}\right) \leq C\|f\|_{L^2(\Omega)}. \tag{1.5.9}$$

□

1.5.2 Lagrangian

Let $z \in H^1(\Omega)$, consider the minimization problem

$$\min_{(u,\Omega)} J(u,\Omega) := \frac{1}{2}\int_\Omega (u(x)-z(x))^2 \mathrm{d}x \text{ under } \begin{cases} -\Delta u = f \text{ in } \Omega, \\ \quad u = 0 \text{ on } \partial\Omega. \end{cases} \tag{1.5.10}$$

The Lagrange function $\mathcal{L} : H_0^1(\Omega) \times H_0^1(\Omega) \times \{\Omega \subset D; \Omega \text{ measurable}\} \to \mathbb{R}$:

$$\mathcal{L}(u,v,\Omega) = J(u,\Omega) + (\nabla u, \nabla v)_{L^2(\Omega)} - (f,v)_{L^2(\Omega)}. \tag{1.5.11}$$

1.5.3 Adjoint equation

We compute the derivative of $\mathcal{L}$ w.r.t. v in the direction $\delta v \in H_0^1(\Omega)$:

$$\mathcal{L}'_v(u,v,\Omega)(\delta v) = (\nabla u, \nabla \delta v)_{L^2(\Omega)} - (f,\delta v)_{L^2(\Omega)} = 0, \ \forall \delta v \in H_0^1(\Omega), \tag{1.5.12}$$

which gives the weak formulation of the state equation $-\Delta u = f$.

We compute the derivative of $\mathcal{L}$ w.r.t. u in the direction $\delta u \in H_0^1(\Omega)$:

$$\mathcal{L}'_u(u,v,\Omega)(\delta u) = (\nabla \delta u, \nabla v)_{L^2(\Omega)} + (u-z,\delta u)_{L^2(\Omega)} = 0, \ \forall \delta u \in H_0^1(\Omega), \tag{1.5.13}$$

which gives the weak formulation of the adjoint equation $-\Delta v = -(u-z)$.

$$\begin{cases} -\Delta v = -(u-z) & \text{in } \Omega, \\ \quad v = 0 & \text{on } \partial\Omega. \end{cases} \tag{1.5.14}$$

Since RHS is in $H^1(\Omega)$, assume additionally $\partial\Omega$ is C^3, we get $v \in H^3(\Omega)$.

1.5.3.1 Boundary representation with local derivatives.

Lemma 1.5.1. *Let $z \in H^1(\Omega)$, $f \in L^2(\Omega)$, $\partial\Omega$ is C^2. The shape derivative of $J(\Omega)$ is given by*

$$dJ(\Omega)[V] = \int_\Gamma \langle V, \mathbf{n}\rangle \left(\frac{1}{2}z^2 - \partial_{\mathbf{n}} u \partial_{\mathbf{n}} v\right) \mathrm{d}s, \tag{1.5.15}$$

Proof. By Theorem 1.5.2, $u, v \in H^2(\Omega)$. Then

$$\begin{aligned} dJ(\Omega)[V] &= \int_\Gamma \langle V,\mathbf{n}\rangle \frac{1}{2}(u-z)^2 \mathrm{d}s + \int_\Omega \left[\frac{1}{2}(u-z)^2\right]' [V]\mathrm{d}x && (1.5.16)\\ &= \int_\Gamma \langle V,\mathbf{n}\rangle \frac{1}{2}z^2 + \int_\Omega (u-z)u'[V]\mathrm{d}x && (1.5.17)\\ &= \int_\Gamma \langle V,\mathbf{n}\rangle \frac{1}{2}z^2 - \int_\Omega \Delta v u'[V]\mathrm{d}x && (1.5.18)\\ &= \int_\Gamma \langle V,\mathbf{n}\rangle \frac{1}{2}z^2 - \int_\Omega v\Delta u'[V]\mathrm{d}x + \int_\Gamma \left(u'[V]\partial_{\mathbf{n}} v - v\frac{\partial u'[V]}{\partial \mathbf{n}}\right) \mathrm{d}s && (1.5.19)\\ &= \int_\Gamma \langle V,\mathbf{n}\rangle \left(\frac{1}{2}z^2 - \partial_{\mathbf{n}} u \partial_{\mathbf{n}} v\right) \mathrm{d}s, && (1.5.20) \end{aligned}$$

where we have used Lemma 1.4.1 in the last equality. □

1.5.3.2 Volume representation with material derivatives

Lemma 1.5.2 (Material derivative and local derivatives)**.** *The following identities hold*

$$d(Du)[V] = D(du[V]) - DuDV, \tag{1.5.21}$$
$$d(\nabla \cdot u)[V] = d(\operatorname{tr}(Du))[V] = \nabla \cdot (du[V]) - \operatorname{tr}(DuDV), \tag{1.5.22}$$

and therefore also immediately if the standard scalar product is used

$$d(\nabla u)[V] = \nabla(du[V]) - (DV)^\top \nabla u \tag{1.5.23}$$

and with the product rule:

$$d\langle \nabla u, \nabla v\rangle[V] = \langle d\nabla u[V], \nabla v\rangle + \langle \nabla u, d\nabla v[V]\rangle = \langle \nabla du[V], \nabla v\rangle + \langle \nabla u, \nabla dv[V]\rangle - \langle \nabla u, (DV + DV^\top)\nabla v\rangle. \tag{1.5.24}$$

Proof. By Remark 1.3.3, one has

$$d(Du)[V] = (Du)'[V] + D(Du)V = D(u'[V]) + D(DuV) - DuDV \tag{1.5.25}$$
$$= D(u'[V] + DuV) - DuDV = D(du[V]) - DuDV. \tag{1.5.26}$$

The part for the div operator follows immediately, because material derivation and $\operatorname{tr}(\cdot)$ are interchangeable, because the trace operator contains no local derivatives. □

Lemma 1.5.3. *Let $z \in L^2(\Omega)$, $f \in L^2(\Omega)$, $\partial\Omega$ is C^2. The shape derivative of $J(\Omega)$ is given by*

$$dJ(u, v, \Omega)[V] = \int_\Omega \frac{1}{2}(u - z)^2 \nabla \cdot V - (u - z)dz[V] - \langle \nabla u, (DV + DV^\top)\nabla v\rangle - vdf[V]\mathrm{d}x. \tag{1.5.27}$$

Proof. We start again with the above Lagrange function again. The shape-directional derivative is given by

$$d\mathcal{L}(u, v, \Omega)[V] = \int_\Omega \operatorname{div}V \left(\frac{1}{2}(u - z)^2 + \langle \nabla u, \nabla v\rangle - vf\right) \mathrm{d}x + \int_\Omega d\left(\frac{1}{2}(u - z)^2 + \langle \nabla u, \nabla v\rangle - vf\right) \mathrm{d}x. \tag{1.5.28}$$

By Theorem 1.5.2, $u \in H^2(\Omega)$. We now use Lemma 1.5.2 and in particular equation (1.5.24) to draw all material derivatives in the last integral:

$$\begin{aligned}&\int_\Omega d\left(\frac{1}{2}(u - z)^2 + \langle \nabla u, \nabla v\rangle - vf\right) \mathrm{d}x \\ &= \int_\Omega (u - z)(du[V] - dz[V]) + \langle \nabla du[V], \nabla v\rangle + \langle \nabla u, \nabla dv[V]\rangle - \langle \nabla u, (DV + DV^\top)\nabla v\rangle - dv[V]f - vdf[V]\mathrm{d}x.\end{aligned} \tag{1.5.29}$$

The following equations hold due to weak formulations of the state and adjoint equations:

$$\langle \nabla u, \nabla dv[V]\rangle - dv[V]f = 0, \tag{1.5.30}$$
$$\langle \nabla du[V], \nabla v\rangle + (u - z)du[V] = 0, \tag{1.5.31}$$

Then (1.5.28) becomes the desired formula. □

Remark 1.5.1. *When comparing (1.5.15) directly with (1.5.27) it is noticeable that in the formulation (1.5.27) the trace of u and ξ is not needed at the boundary. The normal $\mathbf{n}$ is not needed either.*

The regularity requirements:

(i) Boundary formulation (1.5.15): $f \in H^1(\Omega)$, $\partial\Omega$ is C^3, $u, v \in H^3(\Omega)$,

(ii) Volume formulation (1.5.27): $f \in L^2(\Omega)$, $\partial\Omega$ is C^2, $u, v \in H^2(\Omega)$.

1.6 Introduction to Turbulence Models*

For mathematical basis of turbulence modeling, see, e.g., Chacón Rebollo and Lewandowski, 2014, Chap. 3.

1.6.1 Boundary conditions

See, e.g., Gunzburger, 1989; John, 2016. We define $\Gamma_{\mathrm{v}}^{\mathbf{u}}$ and Γ_{v}^{p} as the "varying" components w.r.t. $\mathbf{u}$ and p of Γ, respectively, i.e.,

$$\begin{aligned}
\Gamma_{\mathrm{nv}}^{\mathbf{u}} &:= \{\mathbf{x} \in \Gamma; (\mathbf{Q}(\mathbf{x}, \mathbf{u}+\tilde{\mathbf{u}}, \nabla\mathbf{u}+\nabla\tilde{\mathbf{u}}, p+\tilde{p}, \mathbf{n}, \mathbf{t}) = \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})) \Rightarrow \tilde{\mathbf{u}} = \mathbf{0}\}, \\
\Gamma_{\mathrm{nv}}^{p} &:= \{\mathbf{x} \in \Gamma; (\mathbf{Q}(\mathbf{x}, \mathbf{u}+\tilde{\mathbf{u}}, \nabla\mathbf{u}+\nabla\tilde{\mathbf{u}}, p+\tilde{p}, \mathbf{n}, \mathbf{t}) = \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})) \Rightarrow \tilde{p} = 0\}, \\
\Gamma_{\mathrm{v}}^{\mathbf{u}} &:= \Gamma \backslash \Gamma_{\mathrm{nv}}^{\mathbf{u}}, \ \Gamma_{\mathrm{v}}^{p} := \Gamma \backslash \Gamma_{\mathrm{nv}}^{p}.
\end{aligned}$$

In the case when $\mathbf{Q}$ is linear w.r.t. $\mathbf{u}$ and p, i.e.,

1. Dirichlet boundary condition:

$$\mathbf{u} = \mathbf{g}, \text{ on } \Gamma_{\mathrm{D}}^{\mathbf{u}}. \tag{D-bc}$$

   In particular, $\mathbf{u} = \mathbf{0}$ on solid walls.

   Since $\mathbf{u} = \mathbf{u} + \tilde{\mathbf{u}} = \mathbf{g}$ implies $\tilde{\mathbf{u}} = \mathbf{0}$ for all $\mathbf{x} \in \Gamma_{\mathrm{D}}^{\mathbf{u}}$, one has $\Gamma_{\mathrm{D}}^{\mathbf{u}} \subset \Gamma_{\mathrm{nv}}^{\mathbf{u}}$.

2. Neumann boundary condition:

$$\nu\partial_{\mathbf{n}}\mathbf{u} - p\mathbf{n} = \mathbf{0}, \text{ on } \Gamma_{\mathrm{N}}. \tag{N-bc}$$

   Since $\nu\partial_{\mathbf{n}}(\mathbf{u}+\tilde{\mathbf{u}}) - (p+\tilde{p})\mathbf{n} = \nu\partial_{\mathbf{n}}\mathbf{u} - p\mathbf{n} = \mathbf{0}$ implies $\nu\partial_{\mathbf{n}}\tilde{\mathbf{u}} - \tilde{p}\mathbf{n} = \mathbf{0}$ only and $(\tilde{\mathbf{u}}, \tilde{p})$ can still vary to satisfy this, one has $\Gamma_{\mathrm{N}} \subset \Gamma_{\mathrm{v}}^{\mathbf{u}}$ and $\Gamma_{\mathrm{N}} \subset \Gamma_{\mathrm{v}}^{p}$.

3. Usually on outflow:

$$-p + \alpha\partial_{\mathbf{n}}\mathbf{u}\cdot\mathbf{n} = 0, \ \alpha\partial_{\mathbf{n}}\mathbf{u}\cdot\mathbf{t} = 0.$$

4. Usually on other fixed boundaries of the domain:

$$\mathbf{u}\cdot\mathbf{n} = 0, \ \alpha\partial_{\mathbf{n}}\mathbf{u}\cdot\mathbf{t} = 0.$$

5. On an artificial boundary, e.g., the exit of a canal, or a free surface, a *no-friction condition*:

$$2\nu\varepsilon(\mathbf{u})\mathbf{n} - p\mathbf{n} = \mathbf{0},$$

   may be useful, see, e.g., Maz'ya and Rossmann, 2005; Maz'ya and Rossmann, 2007; Maz'ya and Rossmann, 2009.

6. $\mathbf{u}_{\boldsymbol{\tau}} = \mathbf{h}$, $-p + 2\varepsilon_{\mathbf{n},\mathbf{n}} = \phi$, where $\mathbf{u}_{\mathbf{n}} = \mathbf{u} \cdot \mathbf{n}$ denotes the *normal* and $\mathbf{u}_{\boldsymbol{\tau}} = \mathbf{u} - \mathbf{u}_{\mathbf{n}}\mathbf{n}$ the *tangential component* of $\mathbf{u}$, $\boldsymbol{\varepsilon}_{\mathbf{n}}$ is the vector $\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n}$, $\boldsymbol{\varepsilon}_{\mathbf{n},\mathbf{n}}(\mathbf{u})$ is the normal component and $\boldsymbol{\varepsilon}_{\mathbf{n},\boldsymbol{\tau}}(\mathbf{u})$ the tangential component of $\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u})$.
7. $\mathbf{u}_{\mathbf{n}} = h$, $\boldsymbol{\varepsilon}_{\mathbf{n},\boldsymbol{\tau}} = \phi$.
8. $-p\mathbf{n} + 2\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u}) = \boldsymbol{\phi}$.

Part I

Shape Optimization for Navier-Stokes Equations

Chapter 2

Shape Optimization for Stokes Equations

2.1 Stationary Stokes equations

In this section, we first consider the following general stationary Stokes equations

$$\begin{cases} -\operatorname{diff}(\nu, \mathbf{u}) + \nabla p = \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } \Omega, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\text{bc}}(\mathbf{x}), & \text{on } \Gamma, \end{cases} \tag{gS}$$

where $\operatorname{diff} : \mathbb{R}_{>0} \times \mathbb{R}^N \to \mathbb{R}^N$ is a *diffusive operator* and can take one of the following forms: $\nabla \cdot (\nu \nabla \mathbf{u})$ or $\nabla \cdot (2\nu \boldsymbol{\varepsilon}(\mathbf{u}))$ when the *kinematic viscosity* ν depends on $\mathbf{x}$, and $\nu \Delta \mathbf{u}$ or $2\nu \nabla \cdot \boldsymbol{\varepsilon}(\mathbf{u})$ when ν is a constant. Hence, we have the following variants:

$$\begin{cases} -\nabla \cdot (\nu \nabla \mathbf{u}) + \nabla p = \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } \Omega, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\text{bc}}(\mathbf{x}), & \text{on } \Gamma, \end{cases} \tag{∇-gS}$$

and

$$\begin{cases} -\nabla \cdot (2\nu \boldsymbol{\varepsilon}(\mathbf{u})) + \nabla p = \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } \Omega, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\text{bc}}(\mathbf{x}), & \text{on } \Gamma, \end{cases} \tag{$\boldsymbol{\varepsilon}$-gS}$$

Remark 2.1.1. *When ν is a constant,* (∇-gS) *becomes*

$$\begin{cases} -\nu \Delta \mathbf{u} + \nabla p = \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \textit{in } \Omega, \\ \nabla \cdot \mathbf{u} = f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \textit{in } \Omega, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\text{bc}}(\mathbf{x}), & \textit{on } \Gamma, \end{cases} \tag{∇-S}$$

which can be found commonly in the literature.

If we set

$$P \coloneqq \begin{bmatrix} -\nu\Delta & \nabla \\ \text{div} & 0 \end{bmatrix}, \ u \coloneqq \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix}, \ f \coloneqq \begin{bmatrix} \mathbf{f} \\ f_{\text{div}} \end{bmatrix},$$

then (iS) *can be rewritten in the form of the first equation in* (gnhBVP).

We also need to specify a set of boundary conditions for (gS) via defining the *boundary operators* $(Q_i)_{i=1}^{n_{\rm bc}}$ s.t.

$$Q_i \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = g_i, \text{ on } \Gamma, \ \forall i = 1, \ldots, n_{\rm bc}.$$

2.1.1 Boundary conditions for stationary Stokes equations

See John, 2016, Chap. 4.

2.1.2 Weak and very weak formulations for stationary Stokes equations

We test both sides of the first equation of (gS) with a test function $\mathbf{v} : \mathbb{R}^N \to \mathbb{R}^N$ and those of the second one with a test function $q : \mathbb{R}^N \to \mathbb{R}$ over Ω:

$$\begin{cases} \displaystyle\int_\Omega (-\operatorname{diff}(\nu, \mathbf{u}) + \nabla p) \cdot \mathbf{v} \mathrm{d}\mathbf{x} = \int_\Omega \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \mathbf{v} \mathrm{d}\mathbf{x}, \\ \displaystyle -\int_\Omega q \nabla \cdot \mathbf{u} \mathrm{d}\mathbf{x} = \int_\Omega q f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathrm{d}\mathbf{x}, \end{cases}$$

and then integrate by parts:

- **Case** $\operatorname{diff}(\nu, \mathbf{u}) = \nabla \cdot (\nu \nabla \mathbf{u})$**.** Use the corresponding formulas in Appendix C.2 to obtain

$$\int_\Omega \nu \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma (p\mathbf{n} - \nu \partial_{\mathbf{n}} \mathbf{u}) \cdot \mathbf{v} \mathrm{d}\Gamma = \int_\Omega \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \mathbf{v} \mathrm{d}\mathbf{x}.$$

- **Case** $\operatorname{diff}(\nu, \mathbf{u}) = \nabla \cdot (2\nu \boldsymbol{\varepsilon}(\mathbf{u}))$**.** Also use formulas in Appendix C.2 to obtain

$$\int_\Omega 2\nu \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) - p \nabla \cdot \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma (p\mathbf{n} - 2\nu \boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u})) \cdot \mathbf{v} \mathrm{d}\Gamma = \int_\Omega \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \mathbf{v} \mathrm{d}\mathbf{x}.$$

2.1.3 Cost functions for (gS)

We consider the general cost functional (cost-func-NS) for (gS). Here are some examples from the literature: `[inserting...]`

2.1.4 Lagrangian & extended Lagrangian for (gS)

To derive the adjoint equations for (gS), we first introduce the following *Lagrangian* (see, e.g., Tröltzsch, 2010):

$$\begin{aligned} L(\mathbf{u}, p, \Omega, \mathbf{v}, q) \coloneqq J(\mathbf{u}, p, \Omega) - \int_\Omega & (-\operatorname{diff}(\nu, \mathbf{u}) + \nabla p - \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \cdot \mathbf{v} \\ & + q(\nabla \cdot \mathbf{u} - f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \mathrm{d}\mathbf{x}, \end{aligned} \tag{L-gS}$$

and the following *extended Lagrangian*:

$$\mathcal{L}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) \coloneqq L(\mathbf{u}, p, \Omega, \mathbf{v}, q) - \int_\Gamma (\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\rm bc}) \cdot \mathbf{v}_{\rm bc} \mathrm{d}\Gamma, \tag{$\mathcal{L}$-gS}$$

where $\mathbf{v}, q, \mathbf{u}_{\rm bc}$ are *Lagrange multipliers*.

We also introduce the following "mixed" Lagrangian with a *switching factor* $\delta_{\mathcal{L}} \in \{0, 1\}$:

$$L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) \coloneqq L(\mathbf{u}, p, \Omega, \mathbf{v}, q) - \delta_{\mathcal{L}} \int_\Gamma (\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\rm bc}) \cdot \mathbf{v}_{\rm bc} \mathrm{d}\Gamma. \tag{$L_{\mathcal{L}}$-gS}$$

2.2 Shape optimization problems for (gS)

Here are 3 different shape optimization problems associated with (cost-func-NS), (L-gS), and ($\mathcal{L}$-gS), respectively:

$$\min_{\Omega\in\mathcal{O}_{\rm ad}} J(\mathbf{u},p,\Omega) \text{ s.t. } (\mathbf{u},p) \text{ solves (gS)},$$
$$\min_{\Omega\in\mathcal{O}_{\rm ad}} L(\mathbf{u},p,\Omega,\mathbf{v},q) \text{ s.t. } (\mathbf{u},p) \text{ satisfies } \mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\rm bc}(\mathbf{x}) \text{ on } \Gamma,$$
$$\min_{\Omega\in\mathcal{O}_{\rm ad}} \mathcal{L}(\mathbf{u},p,\Omega,\mathbf{v},q,\mathbf{v}_{\rm bc}) \text{ with } (\mathbf{u},p) \text{ unconstrained},$$

and

$$\min_{\Omega\in\mathcal{O}_{\rm ad}} L_{\mathcal{L}}(\mathbf{u},p,\Omega,\mathbf{v},q,\mathbf{v}_{\rm bc}) \begin{cases} \text{s.t. } (\mathbf{u},p) \text{ satisfies } \mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\rm bc}(\mathbf{x}) \text{ on } \Gamma & \text{if } \delta_{\mathcal{L}}=0,\\ \text{with } (\mathbf{u},p) \text{ unconstrained} & \text{if } \delta_{\mathcal{L}}=1.\end{cases}$$

Choose the adjoint variables/Lagrangian multipliers $(\mathbf{v},q,\mathbf{v}_{\rm bc})$ s.t.

$$D_{\mathbf{u}}L_{\mathcal{L}}(\mathbf{u},p,\Omega,\mathbf{v},q,\mathbf{v}_{\rm bc})\tilde{\mathbf{u}} + D_pL_{\mathcal{L}}(\mathbf{u},p,\Omega,\mathbf{v},q,\mathbf{v}_{\rm bc})\tilde{p} = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}).$$

Expand this more explicitly for all $(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p})$:

$$\begin{aligned}
&\int_\Omega D_{\mathbf{u}}\left(J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\tilde{\mathbf{u}} + D_p\left(J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\tilde{p}\mathrm{d}\mathbf{x}\\
&+\int_\Gamma D_{\mathbf{u}}\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right)\tilde{\mathbf{u}} + D_p\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right)\tilde{p}\mathrm{d}\Gamma\\
&-\int_\Omega \left[-D_{\mathbf{u}}(\mathrm{diff}(\nu,\mathbf{u}))\tilde{\mathbf{u}} - D_{\mathbf{u}}(f(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\tilde{\mathbf{u}} + \nabla\tilde{p} - D_pf(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\right]\cdot\mathbf{v}\\
&\qquad + q\left[\nabla\cdot\tilde{\mathbf{u}} - D_{\mathbf{u}}(f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\tilde{\mathbf{u}} - D_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\right]\mathrm{d}\mathbf{x}\\
&-\delta_{\mathcal{L}}\int_\Gamma \left[D_{\mathbf{u}}(Q(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}))\tilde{\mathbf{u}} + D_pQ(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{p}\right]\cdot\mathbf{v}_{\rm bc}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}),
\end{aligned}$$

and more explicitly:

$$\begin{aligned}
&\int_\Omega D_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}} + D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}} + D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\mathrm{d}\mathbf{x}\\
&+\int_\Gamma D_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{\mathbf{u}} + D_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}} + D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{p}\mathrm{d}\Gamma\\
&+\int_\Omega D_{\mathbf{u}}(\mathrm{diff}(\nu,\mathbf{u}))\tilde{\mathbf{u}}\cdot\mathbf{v} + D_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\cdot\mathbf{v} + D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v} - \nabla\tilde{p}\cdot\mathbf{v}\\
&\qquad + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\cdot\mathbf{v} - q\nabla\cdot\tilde{\mathbf{u}} + qD_{\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\\
&\qquad + qD_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}} + qD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\mathrm{d}\mathbf{x}\\
&-\delta_{\mathcal{L}}\int_\Gamma D_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc} + D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc}\\
&\qquad + D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{p}\cdot\mathbf{v}_{\rm bc}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}),
\end{aligned}$$

where

$$D_{\mathbf{u}}(\mathrm{diff}(\nu,\mathbf{u}))\tilde{\mathbf{u}} = \begin{cases}\nabla\cdot(\nu\nabla\tilde{\mathbf{u}}), & \text{if } \mathrm{diff}(\nu,\mathbf{u}) = \nabla\cdot(\nu\nabla\mathbf{u}),\\ \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\tilde{\mathbf{u}})), & \text{if } \mathrm{diff}(\nu,\mathbf{u}) = \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{u})).\end{cases}$$

Integrating by parts all the terms whose integrands are: $D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}$, $D_{\mathbf{u}}(\mathrm{diff}(\nu,\mathbf{u}))\tilde{\mathbf{u}}\cdot\mathbf{v}$, $D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}$, $-\nabla\tilde{p}\cdot\mathbf{v}$, $-q\nabla\cdot\tilde{\mathbf{u}}$, $qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}$[1] yields:

1. **Case 1:** $\mathrm{diff}(\nu,\mathbf{u}) = \nabla\cdot(\nu\nabla\mathbf{u})$.

$$
\begin{aligned}
&\int_\Omega \big[\nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) + \nabla\cdot(\nu\nabla\mathbf{v}) + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v}\\
&\qquad - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\mathbf{v} + \nabla q + q\nabla_{\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\\
&\qquad - D_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla q - q(\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)))\big]\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}\\
&+\int_\Omega \tilde{p}\left[D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \nabla\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_pf_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right]\mathrm{d}\mathbf{x}\\
&+\int_\Gamma \big[D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \nu\partial_{\mathbf{n}}\mathbf{v} + ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v}) - q\mathbf{n}\\
&\qquad + qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} - \delta_{\mathcal{L}}\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\mathrm{bc}}\big]\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma\\
&+\int_\Gamma \tilde{p}\left[D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{v}\cdot\mathbf{n} - \delta_{\mathcal{L}}D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\mathrm{bc}}\right]\mathrm{d}\Gamma\\
&+\int_\Gamma D_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}} + \nu\partial_{\mathbf{n}}\tilde{\mathbf{u}}\cdot\mathbf{v} - \delta_{\mathcal{L}}D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\mathrm{bc}}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}).
\end{aligned}
\tag{EL-gS1}
$$

We consider the following subcases:

- **Case 1.1:** $\delta_{\mathcal{L}} = 0$. This means to "activate" the boundary-condition constraint $\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x})$ on Γ, so it will not be penalized by the Lagrangian L.
To see the general structure, we rewrite (EL-gS1) as follows:

$$
\begin{aligned}
&\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},\Delta\mathbf{v},q,\nabla q)\cdot\tilde{\mathbf{u}} + F_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\nabla\mathbf{v},q)\tilde{p}\mathrm{d}\mathbf{x}\\
&+\int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{n},\mathbf{t})\cdot\tilde{\mathbf{u}} + F_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\mathbf{n},\mathbf{t})\tilde{p}\\
&\qquad + \mathbf{F}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\mathbf{n},\mathbf{t}):\nabla\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}),
\end{aligned}
\tag{brEL-gS1.1}
$$

where

$$
\begin{aligned}
&\mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},\Delta\mathbf{v},q,\nabla q)\\
&\quad\coloneqq \nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) + \nabla\cdot(\nu\nabla\mathbf{v}) + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v}\\
&\qquad - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\mathbf{v} + \nabla q + q\nabla_{\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\\
&\qquad - D_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla q - q(\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))),\\
&F_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\nabla\mathbf{v},q) \coloneqq D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \nabla\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_pf_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p),\\
&\mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{n},\mathbf{t})\\
&\quad\coloneqq D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \nu\partial_{\mathbf{n}}\mathbf{v} + ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v})\\
&\qquad - q\mathbf{n} + qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n},\\
&F_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\mathbf{n},\mathbf{t}) \coloneqq D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{v}\cdot\mathbf{n},\\
&\mathbf{F}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{v},\mathbf{n},\mathbf{t},\nabla\tilde{\mathbf{u}}) \coloneqq \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nu\mathbf{n}\otimes\mathbf{v},
\end{aligned}
$$

are defined for all $(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{n},\mathbf{t},\tilde{\mathbf{u}},\tilde{p})$.
To proceed further, we need the following "separation" lemma.

[1] Look up Appendix C.2.

Lemma 2.2.1 (Separation argument)**.** *Suppose that the mappings*

$$
\begin{aligned}
\mathbf{I}_\Omega^{\tilde{\mathbf{u}}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}^N, \\
I_\Omega^{\tilde{p}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}, \\
\mathbf{I}_\Gamma^{\tilde{\mathbf{u}}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^{N(N-1)} \to \mathbb{R}^N, \\
I_\Gamma^{\tilde{p}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^{N(N-1)} \to \mathbb{R}, \\
\mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^{N(N-1)} \to \mathbb{R}^{N^2},
\end{aligned}
$$

satisfy the integral equation

$$
\begin{aligned}
&\int_\Omega \mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) \cdot \tilde{\mathbf{u}} + I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q)\tilde{p} \mathrm{d}\mathbf{x} \\
&+ \int_\Gamma \mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} + I_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t})\tilde{p} + \mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,
\end{aligned}
\tag{2.2.1}
$$

for all $(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p})$ *satisfying*

$$
\mathbf{Q}(\mathbf{x}, \mathbf{u} + \tilde{\mathbf{u}}, \nabla\mathbf{u} + \nabla\tilde{\mathbf{u}}, p + \tilde{p}, \mathbf{n}, \mathbf{t}) = \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x}) \ \textit{on } \Gamma. \tag{2.2.2}
$$

Then

$$
\begin{cases}
\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) = \mathbf{0}, & \textit{in } \Omega, \\
I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) = 0, & \textit{in } \Omega, \\
\mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) = \mathbf{0}, & \textit{on } \Gamma_{\mathrm{v}}^{\mathbf{u}}, \\
I_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) = 0, & \textit{on } \Gamma_{\mathrm{v}}^{p}, \\
\mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) = \mathbf{0}_{N\times N}, & \textit{on } \Gamma.
\end{cases}
\tag{2.2.3}
$$

Proof. Choosing $\tilde{\mathbf{u}} = \mathbf{0}$ in $\overline{\Omega}$, then $\nabla\tilde{\mathbf{u}} = \mathbf{0}_{N\times N}$ on Γ and (2.2.1) becomes

$$
\int_\Omega I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q)\tilde{p} \mathrm{d}\mathbf{x} + \int_\Gamma I_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t})\tilde{p} \mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{p}) \text{ s.t. } (2.2.2). \tag{2.2.4}
$$

Then choosing $\tilde{p}$ varying such that $\tilde{p}|_\Gamma = 0$, the last equation gives

$$
\int_\Omega I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q)\tilde{p} \mathrm{d}\mathbf{x} = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{p}) \text{ s.t. } (2.2.2), \ \tilde{p}|_\Gamma = 0.
$$

Hence, the integrand must vanish identically, i.e., $(\mathbf{v}, q)$ must satisfy

$$
I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) = 0, \text{ in } \Omega. \tag{2.2.5}
$$

Plug (2.2.5) back in (2.2.4), we obtain

$$
\int_\Gamma I_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t})\tilde{p} \mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{p}) \text{ s.t. } (2.2.2).
$$

Since $\tilde{p}|_{\Gamma_{\mathrm{nv}}^p} = 0$, the last equation implies that $(\mathbf{v}, q)$ must satisfy

$$
I_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) = 0, \text{ on } \Gamma_{\mathrm{v}}^p. \tag{2.2.6}
$$

Assume $(\mathbf{v}, q)$ satisfies (2.2.5) and (2.2.6), then (2.2.1) becomes, for all $(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}})$ satisfying (2.2.2),

$$\int_\Omega \mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} + \mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} \mathrm{d}\Gamma = 0. \tag{2.2.7}$$

Choosing $\tilde{\mathbf{u}}$ varying such that $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$ and $\nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}$ in (2.2.7) yields

$$\int_\Omega \mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} = 0,\ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } (2.2.2),\ \tilde{\mathbf{u}}|_\Gamma = \mathbf{0},\ \nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}.$$

Hence, $(\mathbf{v}, q)$ satisfies

$$\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) = \mathbf{0},\ \text{in } \Omega. \tag{2.2.8}$$

Plug (2.2.8) back in (2.2.7) to obtain

$$\int_\Gamma \mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_\Gamma \mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,\ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } (2.2.2).$$

Since $\tilde{\mathbf{u}}|_{\Gamma_{\mathrm{nv}}^{\mathbf{u}}} = \mathbf{0}$, the last equation yields

$$\int_{\Gamma_{\mathrm{v}}^{\mathbf{u}}} \mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_\Gamma \mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,\ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } (2.2.2). \tag{2.2.9}$$

Choosing $\tilde{\mathbf{u}}$ varying such that $\tilde{\mathbf{u}} = \mathbf{0}$ on $\Gamma_{\mathrm{v}}^{\mathbf{u}}$, then (2.2.9) becomes

$$\int_\Gamma \mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,\ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } (2.2.2),\ \tilde{\mathbf{u}} = \mathbf{0},$$

which implies that $\mathbf{v}$ must satisfy

$$\mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) = \mathbf{0}_{N\times N},\ \text{on } \Gamma. \tag{2.2.10}$$

Plug (2.2.10) back in (2.2.9) to obtain

$$\int_{\Gamma_{\mathrm{v}}^{\mathbf{u}}} \mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,\ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } (2.2.2),$$

which implies that $(\mathbf{v}, q)$ must satisfy

$$\mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{n}, \mathbf{t}) = \mathbf{0},\ \text{on } \Gamma_{\mathrm{v}}^{\mathbf{u}}. \tag{2.2.11}$$

Gathering (2.2.5), (2.2.6), (2.2.8), (2.2.10), and (2.2.11) yields (2.2.3). □

Now applying Lemma 2.2.1 with $(\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}, I_\Omega^{\tilde{p}}, \mathbf{I}_\Gamma^{\tilde{\mathbf{u}}}, I_\Gamma^{\tilde{p}}, \mathbf{I}_\Gamma^{\nabla\tilde{\mathbf{u}}}) = (\mathbf{F}_\Omega^{\tilde{\mathbf{u}}}, F_\Omega^{\tilde{p}}, \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}, F_\Gamma^{\tilde{p}}, \mathbf{F}_\Gamma^{\nabla\tilde{\mathbf{u}}})$ yields the following adjoint equation for (gS):

$$\begin{cases} \nabla\cdot(\nu\nabla\mathbf{v}) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) : \nabla\mathbf{v} + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\mathbf{v} - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p))\cdot\mathbf{v} \\ \quad + (1 - D_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p))\nabla q + q[\nabla_{\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) - (\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)))] \\ \qquad = -\nabla_{\mathbf{u}}J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) + \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)),\ \text{in } \Omega, \\ \nabla\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\cdot\mathbf{v} + qD_pf_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) = -D_pJ_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p),\ \text{in } \Omega, \\ -\nu\partial_{\mathbf{n}}\mathbf{v} + ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\cdot\mathbf{n})\cdot\mathbf{v}) + q(D_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) - 1)\mathbf{n} \\ \qquad = -D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\mathbf{n} - \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}),\ \text{on } \Gamma_{\mathrm{v}}^{\mathbf{u}}, \\ \mathbf{v}\cdot\mathbf{n} = D_pJ_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}),\ \text{on } \Gamma_{\mathrm{v}}^{p}, \\ \nu\mathbf{n}\otimes\mathbf{v} = -\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}),\ \text{on } \Gamma. \end{cases} \tag{adj-gS1.1}$$

Question 2.2.1. *Is* (adj-gS1.1) *overdetermined or underdetermined? If yes, in which cases of the cost functional* J*?*

- **Case 1.2:** $\delta_{\mathcal{L}} = 1$**.** This means to "deactivate" the boundary-condition constraint $\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x})$ on Γ, so it will be penalized by the extended Lagrangian $\mathcal{L}$.
Again, to see the general structure, we rewrite (EL-gS1) as follows:

$$\begin{aligned}
&\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p, \mathbf{v}, \nabla \mathbf{v}, \Delta \mathbf{v}, q, \nabla q) \cdot \tilde{\mathbf{u}} + F_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \nabla \mathbf{v}, q)\tilde{p} \mathrm{d}\mathbf{x} \\
&+ \int_\Gamma \boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \nabla \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} + \mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t})\tilde{p} \\
&\qquad + \boldsymbol{\mathcal{F}}_\Gamma^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) : \nabla \tilde{\mathbf{u}} \mathrm{d}\Gamma = 0, \;\; \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p}),
\end{aligned} \tag{brEL-gS1.2}$$

where

$$\begin{aligned}
\boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \nabla \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) &\coloneqq \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \nabla \mathbf{v}, q, \mathbf{n}, \mathbf{t}) - \nabla_{\mathbf{u}} \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \mathbf{v}_{\mathrm{bc}}, \\
\mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) &\coloneqq F_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) - D_p \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{v}_{\mathrm{bc}}, \\
\boldsymbol{\mathcal{F}}_\Gamma^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) &\coloneqq \mathbf{F}_\Gamma^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{v}, \mathbf{n}, \mathbf{t}) - \nabla_{\nabla \mathbf{u}} \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{v}_{\mathrm{bc}}.
\end{aligned}$$

Note the the domain integrands are the same as the standard-Lagrangian case, only the boundary integrands are modified with the additional Lagrange multiplier $\mathbf{v}_{\mathrm{bc}}$ in this extended-Lagrangian case.

Lemma 2.2.2 (Separation argument)**.** *Suppose that the mappings* $\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}$, $I_\Omega^{\tilde{p}}$, $\boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}$, $\mathcal{I}_\Gamma^{\tilde{p}}$, *and* $\mathcal{I}_\Gamma^{\nabla \tilde{\mathbf{u}}}$ *satisfy*

$$\begin{aligned}
\mathbf{I}_\Omega^{\tilde{\mathbf{u}}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}^N, \\
I_\Omega^{\tilde{p}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}, \\
\boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^{N(N-1)} \to \mathbb{R}^N, \\
\mathcal{I}_\Gamma^{\tilde{p}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^{N(N-1)} \to \mathbb{R}, \\
\boldsymbol{\mathcal{I}}_\Gamma^{\nabla \tilde{\mathbf{u}}} &: \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^{N(N-1)} \to \mathbb{R}^{N^2},
\end{aligned}$$

satisfy the integral equation

$$\begin{aligned}
&\int_\Omega \mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) \cdot \tilde{\mathbf{u}} + I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q)\tilde{p} \mathrm{d}\mathbf{x} \\
&+ \int_\Gamma \boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} + \mathcal{I}_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t})\tilde{p} + \boldsymbol{\mathcal{I}}_\Gamma^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) : \nabla \tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,
\end{aligned} \tag{2.2.12}$$

for all $(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p})$*. Then*

$$\begin{cases}
\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) = \mathbf{0}, & \textit{in } \Omega, \\
I_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q) = 0, & \textit{in } \Omega, \\
\boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) = \mathbf{0}, & \textit{on } \Gamma, \\
\mathcal{I}_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, q, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) = 0, & \textit{on } \Gamma, \\
\boldsymbol{\mathcal{I}}_\Gamma^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, p, \mathbf{v}, \mathbf{v}_{\mathrm{bc}}, \mathbf{n}, \mathbf{t}) = \mathbf{0}_{N \times N}, & \textit{on } \Gamma.
\end{cases} \tag{2.2.13}$$

Proof. Choosing $\tilde{\mathbf{u}} = \mathbf{0}$ in $\overline{\Omega}$, then $\nabla\tilde{\mathbf{u}} = \mathbf{0}_{N\times N}$ on Γ and (2.2.12) becomes

$$\int_\Omega I_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q)\tilde{p}\mathrm{d}\mathbf{x} + \int_\Gamma \mathcal{I}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t})\tilde{p}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{p}). \tag{2.2.14}$$

Then choosing $\tilde{p}$ varying such that $\tilde{p}|_\Gamma = 0$, the last equation gives

$$\int_\Omega I_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q)\tilde{p}\mathrm{d}\mathbf{x} = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{p}) \text{ s.t. } \tilde{p}|_\Gamma = 0.$$

Hence, the integrand must vanish identically, i.e., $(\mathbf{v},q)$ must satisfy

$$I_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q) = 0,\ \text{ in } \Omega. \tag{2.2.15}$$

Plug (2.2.15) back in (2.2.14), we obtain

$$\int_\Gamma \mathcal{I}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t})\tilde{p}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{p}),$$

which implies that $(\mathbf{v},q)$ must satisfy

$$\mathcal{I}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) = 0,\ \text{ on } \Gamma. \tag{2.2.16}$$

Assume $(\mathbf{v},q)$ satisfies (2.2.15) and (2.2.16), then (2.2.12) becomes, for all $(\mathbf{u},p,\Omega,\tilde{\mathbf{u}})$,

$$\int_\Omega \mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q)\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma \boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t})\cdot\tilde{\mathbf{u}} + \boldsymbol{\mathcal{I}}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) : \nabla\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0. \tag{2.2.17}$$

Choosing $\tilde{\mathbf{u}}$ varying such that $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$ and $\nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}$ in (2.2.17) yields

$$\int_\Omega \mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q)\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}) \text{ s.t. } \tilde{\mathbf{u}}|_\Gamma = \mathbf{0},\ \nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N},$$

which implies that $(\mathbf{v},q)$ must satisfy

$$\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q) = \mathbf{0},\ \text{ in } \Omega. \tag{2.2.18}$$

Plug (2.2.18) back in (2.2.17) to obtain

$$\int_\Gamma \boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t})\cdot\tilde{\mathbf{u}} + \boldsymbol{\mathcal{I}}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) : \nabla\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}). \tag{2.2.19}$$

Choosing $\tilde{\mathbf{u}}$ varying such that $\tilde{\mathbf{u}} = \mathbf{0}$ on Γ, then (2.2.19) becomes

$$\int_\Gamma \boldsymbol{\mathcal{I}}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) : \nabla\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}) \text{ s.t. } \tilde{\mathbf{u}} = \mathbf{0},$$

which implies that $\mathbf{v}$ must satisfy

$$\boldsymbol{\mathcal{I}}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) = \mathbf{0}_{N\times N},\ \text{ on } \Gamma. \tag{2.2.20}$$

Plug (2.2.20) back in (2.2.19) to obtain

$$\int_\Gamma \boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t})\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}).$$

which implies that $(\mathbf{v},q)$ must satisfy

$$\boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) = \mathbf{0},\ \text{ on } \Gamma. \tag{2.2.21}$$

Gathering (2.2.15), (2.2.16), (2.2.18), (2.2.20), and (2.2.21) yields (2.2.13). □

Now applying Lemma 2.2.2 with $(\mathbf{I}_\Omega^{\tilde{\mathbf{u}}}, I_\Omega^{\tilde{p}}, \boldsymbol{\mathcal{I}}_\Gamma^{\tilde{\mathbf{u}}}, \mathcal{I}_\Gamma^{\tilde{p}}, \boldsymbol{\mathcal{I}}_\Gamma^{\nabla\tilde{\mathbf{u}}}) = (\mathbf{F}_\Omega^{\tilde{\mathbf{u}}}, F_\Omega^{\tilde{p}}, \boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}, \mathcal{F}_\Gamma^{\tilde{p}}, \boldsymbol{\mathcal{F}}_\Gamma^{\nabla\tilde{\mathbf{u}}})$ yields the following adjoint equation for (gS):

$$\begin{cases} \nabla\cdot(\nu\nabla\mathbf{v}) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v} + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v} - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} \\ \quad + (1 - D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\nabla q + q[\nabla_{\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - (\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)))] \\ \qquad = -\nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)), \text{ in } \Omega, \\ \nabla\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) = -D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p), \text{ in } \Omega, \\ -\nu\partial_{\mathbf{n}}\mathbf{v} + ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v}) + q(D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - 1)\mathbf{n} - \nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\rm bc} \\ \qquad = -D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} - \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}), \text{ on } \Gamma, \\ \mathbf{v}\cdot\mathbf{n} - D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\rm bc} = D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}), \text{ on } \Gamma, \\ \nu\mathbf{n}\otimes\mathbf{v} - \nabla_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\rm bc} = -\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}), \text{ on } \Gamma. \end{cases} \tag{adj-gS1.2}$$

2. **Case 2:** $\operatorname{diff}(\nu,\mathbf{u}) = \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{u}))$.

$$\begin{aligned} &\int_\Omega [\nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) + \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v})) + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v} \\ &\quad - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v} + \nabla q + q\nabla_{\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \\ &\quad - D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla q - q(\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)))]\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} \\ &+ \int_\Omega \tilde{p}\,[D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \nabla\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathrm{d}\mathbf{x} \\ &+ \int_\Gamma [D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - 2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{v}) + ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v}) - q\mathbf{n} \\ &\qquad + qD_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} - \delta_{\mathcal{L}}\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\rm bc}]\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma \\ &+ \int_\Gamma \tilde{p}\,[D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{v}\cdot\mathbf{n} - \delta_{\mathcal{L}}D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\rm bc}]\,\mathrm{d}\Gamma \\ &+ \int_\Gamma D_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}} + 2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\tilde{\mathbf{u}})\cdot\mathbf{v} - \delta_{\mathcal{L}}D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc}\mathrm{d}\Gamma = 0, \ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}). \end{aligned}$$

Note that only the following three terms are changed compared to the previous case:

$$\begin{aligned} &\int_\Omega \nabla\cdot(\nu\nabla\mathbf{v})\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}, \ \int_\Gamma -\nu\partial_{\mathbf{n}}\mathbf{v}\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma, \ \int_\Gamma \nu\partial_{\mathbf{n}}\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\Gamma \text{ are replaced by} \\ &\int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v}))\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}, \ \int_\Gamma -2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{v})\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma, \ \int_\Gamma 2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\tilde{\mathbf{u}})\cdot\mathbf{v}\mathrm{d}\Gamma. \end{aligned}$$

- **Case 1.1:** $\delta_{\mathcal{L}} = 0$. Similarly, we obtain the following adjoint equation for (gS):

$$\begin{cases} \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v})) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v} + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v} - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} \\ \quad + (1 - D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\nabla q + q[\nabla_{\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - (\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)))] \\ \qquad = -\nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)), \text{ in } \Omega, \\ \nabla\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) = -D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p), \text{ in } \Omega, \\ -2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{v}) + ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v}) + q(D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - 1)\mathbf{n} \\ \qquad = -D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n} - \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}), \text{ on } \Gamma_{\rm v}^{\mathbf{u}}, \\ \mathbf{v}\cdot\mathbf{n} = D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}), \text{ on } \Gamma_{\rm v}^{p}, \\ \nu(\mathbf{n}\otimes\mathbf{v} + \mathbf{v}\otimes\mathbf{n}) = -\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}), \text{ on } \Gamma. \end{cases} \tag{adj-gS2.1}$$

where in the last equation we have used the following to deduce,

$$\begin{aligned}2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\tilde{\mathbf{u}})\cdot\mathbf{v} &= 2\nu\mathbf{n}^\top\boldsymbol{\varepsilon}(\tilde{\mathbf{u}})\mathbf{v} = \nu\mathbf{n}^\top(\nabla\tilde{\mathbf{u}}+D\tilde{\mathbf{u}})\mathbf{v} = \nu(\mathbf{n}^\top\nabla\tilde{\mathbf{u}}\mathbf{v}+\mathbf{n}^\top D\tilde{\mathbf{u}}\mathbf{v})\\ &= \nu(\mathbf{n}^\top\nabla\tilde{\mathbf{u}}\mathbf{v}+\mathbf{v}^\top\nabla\tilde{\mathbf{u}}\mathbf{n}) = \nu(\mathbf{n}\otimes\mathbf{v}+\mathbf{v}\otimes\mathbf{n}):\nabla\tilde{\mathbf{u}}.\end{aligned}$$

Case 1.2: $\delta_{\mathcal{L}}=1$**.** Similarly, we obtain the following adjoint equation for (gS):

$$\begin{cases}\nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v}))-\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\mathbf{v}+\nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v}-\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v}\\ \quad+(1-D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\nabla q+q[\nabla_{\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)-(\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)))]\\ \qquad=-\nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)+\nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)),\ \text{in }\Omega,\\ \nabla\cdot\mathbf{v}+D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v}+qD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)=-D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p),\ \text{in }\Omega,\\ -2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{v})+((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v})+q(D_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)-1)\mathbf{n}-\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\rm bc}\\ \qquad=-D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n}-\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}),\ \text{on }\Gamma,\\ \mathbf{v}\cdot\mathbf{n}-D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\rm bc}=D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}),\ \text{on }\Gamma,\\ \nu(\mathbf{n}\otimes\mathbf{v}+\mathbf{v}\otimes\mathbf{n})-\nabla_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\rm bc}=-\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}),\ \text{on }\Gamma.\end{cases}\tag{adj-gS2.2}$$

2.2.1 Shape derivatives of (gS)-constrained (cost-func-NS)

To calculate the shape derivatives of (cost-func-NS) under the constraint state equation (gS), we consider the following *perturbed cost functional*

$$J(\mathbf{u}_t,p_t,\Omega_t):=\int_{\Omega_t}J_\Omega(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t)\mathrm{d}\mathbf{x}+\int_{\Gamma_t}J_\Gamma(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t,\mathbf{n}_t,\mathbf{t}_t)\mathrm{d}\Gamma_t,\tag{2.2.22}$$

where $(\mathbf{u}_t,p_t)$ denotes the strong/classical solution of (gS) on the perturbed domain $\Omega_t:=T_t(V)(\Omega)$, i.e.:

$$\begin{cases}-\nu\Delta\mathbf{u}_t+\nabla p_t=\mathbf{f} & \text{in }\Omega_t,\\ \nabla\cdot\mathbf{u}_t=f_{\rm div} & \text{in }\Omega_t,\\ \gamma_0\mathbf{u}_t=\mathbf{u}_\Gamma\text{ i.e., }\mathbf{u}_t=\mathbf{u}_\Gamma & \text{on }\Gamma_t,\end{cases}\tag{ptb-S}$$

where $\Gamma_t:=\partial\Omega_t$.

Now subtracting (ptb-S) to (gS) side by side, and taking $\lim_{t\downarrow 0}$, obtain:

2.2.2 Existence, uniqueness, and regularity

We consider the following stationary Stokes equations:

$$\begin{cases}-\nu\Delta\mathbf{u}+\nabla p=\mathbf{f}, & \text{in }\Omega,\\ \nabla\cdot\mathbf{u}=f_{\rm div}, & \text{in }\Omega,\\ \gamma_0\mathbf{u}=\mathbf{u}_\Gamma\text{ i.e., }\mathbf{u}=\mathbf{u}_\Gamma, & \text{on }\Gamma,\end{cases}\tag{S}$$

where $\gamma_0\in\mathcal{L}(H^1(\Omega),L^2(\Gamma))$ is the trace operator s.t. $\gamma_0 u=$ the restriction of u to Γ for every function $u\in H^1(\Omega)$ (see, e.g., Temam, 2000, p. 6).

Theorem 2.2.1 (Case $f_{\rm div}=0$, $\mathbf{u}_\Gamma=\mathbf{0}$)**.** *(i) (Existence) For any open set $\Omega\subset\mathbb{R}^N$ which is bounded in some direction, and for every $\mathbf{f}\in\mathbf{H}^{-1}(\Omega)$, the problem*

$$\mathbf{u}\text{ belongs to }V\text{ and satisfies }\nu((\mathbf{u},\mathbf{v}))=\langle\mathbf{f},\mathbf{v}\rangle_{V^\star,V},\ \forall\mathbf{v}\in V\tag{2.2.23}$$

has a unique solution $\mathbf{u}$.

Moreover, there exists a function $p\in L^2_{\rm loc}(\Omega)$ s.t. the following 2 statements are satisfied:

(a) there exists $p \in L^2(\Omega)$ *s.t.* $-\nu\Delta\mathbf{u} + \nabla p = \mathbf{f}$ *in the distribution sense in* Ω*;*

(b) $\nabla\cdot\mathbf{u} = 0$ *in the distribution sense in* Ω*.*

If Ω *is an open bounded set of class* C^2*, then* $p \in L^2(\Omega)$ *and (a), (b), and* $\gamma_0\mathbf{u} = \mathbf{0}$ *are satisfied by* $\mathbf{u}$ *and* p*.*

(ii) (A variational property) The solution $\mathbf{u}$ *of* (2.2.23) *is also the unique element of* V *s.t.*

$$E(\mathbf{u}) \le E(\mathbf{v}),\ \forall\mathbf{v}\in V,\ \textit{where } E(\mathbf{v}) \coloneqq \nu\|\mathbf{v}\|^2 - 2\langle\mathbf{f},\mathbf{v}\rangle_{V^\star,V}.$$

Theorem 2.2.2 (Non-homogeneous Stokes: Existence)**.** *(i) Let* Ω *be an open bounded set of class* C^2 *in* $\mathbb{R}^N$*. Let there be given* $\mathbf{f}\in\mathbf{H}^{-1}(\Omega)$*,* $f_{\text{div}}\in L^2(\Omega)$*,* $\mathbf{u}_\Gamma\in\mathbf{H}^{1/2}(\Gamma)$*, s.t.*

$$\int_\Omega f_{\text{div}}\mathrm{d}\mathbf{x} = \int_\Gamma \mathbf{u}_\Gamma\cdot\mathbf{n}\mathrm{d}\Gamma.$$

Then there exists $\mathbf{u}\in\mathbf{H}^1(\Omega)$*,* $p\in L^2(\Omega)$*, which are solution of the non-homogeneous Stokes problem* (S)*,* $\mathbf{u}$ *is unique and* p *is unique up to the addition of a constant.*

(ii) Let Ω *be a Lipschitz open bounded set in* $\mathbb{R}^N$*. Let there be given* $\mathbf{f}\in\mathbf{H}^{-1}(\Omega)$*,* $f_{\text{div}}\in L^2(\Omega)$*,* $\mathbf{u}_\Gamma$ *as the trace of a function* $\mathbf{u}_{\Gamma,0}\in\mathbf{H}^1(\Omega)$*, s.t.*

$$\int_\Omega f_{\text{div}}\mathrm{d}\mathbf{x} = \int_\Omega \nabla\cdot\mathbf{u}_{\Gamma,0}\mathrm{d}\mathbf{x}.$$

Then there exists $\mathbf{u}\in\mathbf{H}^1(\Omega)$*,* $p\in L^2(\Omega)$*, which are solution of the non-homogeneous Stokes problem*

$$\begin{cases} -\nu\Delta\mathbf{u} + \nabla p = \mathbf{f} & \textit{in } \Omega,\\ \nabla\cdot\mathbf{u} = f_{\text{div}} & \textit{in } \Omega,\\ \mathbf{u} - \mathbf{u}_{\Gamma,0} \in \mathbf{H}^1_0(\Omega). & \end{cases}$$

$\mathbf{u}$ *is unique and* p *is unique up to the addition of a constant.*

Theorem 2.2.3 (Non-homogeneous Stokes: regularity)**.** *(i) Let* Ω *be an open bounded set of class* C^r*,* $r = \max(m+2,2)$*,* m *integer* > 0*. Let us suppose that* $\mathbf{u}\in\mathbf{W}^{2,\alpha}(\Omega)$*,* $p\in W^{1,\alpha}(\Omega)$*,* $1<\alpha<+\infty$*, are solutions of the generalized Stokes problem*

$$\begin{cases} -\nu\Delta\mathbf{u} + \nabla p = \mathbf{f} & \textit{in } \Omega,\\ \nabla\cdot\mathbf{u} = f_{\text{div}} & \textit{in } \Omega,\\ \gamma_0\mathbf{u} = \mathbf{u}_\Gamma \textit{ i.e., } \mathbf{u} = \mathbf{u}_\Gamma & \textit{on } \Gamma, \end{cases}$$

If $\mathbf{u}\in\mathbf{W}^{m,\alpha}(\Omega)$*,* $f_{\text{div}}\in W^{m+1,\alpha}(\Omega)$ *and* $\mathbf{u}_\Gamma\in\mathbf{W}^{m+2-1/\alpha,\alpha}(\Gamma)$*,*[2] *then* $\mathbf{u}\in\mathbf{W}^{m+2,\alpha}(\Omega)$*,* $p\in W^{m+1,\alpha}(\Omega)$ *and there exists a constant* $c_0(\alpha,\nu,m,\Omega)$ *s.t.*

$$\begin{aligned} &\|\mathbf{u}\|_{\mathbf{W}^{m+2,\alpha}(\Omega)} + \|p\|_{W^{m+1,\alpha}(\Omega)/\mathbb{R}}\\ &\le c_0\left\{\|\mathbf{f}\|_{\mathbf{W}^{m,\alpha}(\Omega)} + \|f_{\text{div}}\|_{W^{m+1,\alpha}(\Omega)} + \|\mathbf{u}_\Gamma\|_{\mathbf{W}^{m+2-1/\alpha,\alpha}(\Gamma)} + d_\alpha\|\mathbf{u}\|_{\mathbf{L}^\alpha(\Omega)}\right\}, \end{aligned} \tag{2.2.24}$$

where $d_\alpha = 0$ *for* $\alpha\ge 2$*,* $d_\alpha = 1$ *for* $1<\alpha<2$*.*

[2] $W^{m+2-1/\alpha,\alpha}(\Gamma) = \gamma_0 W^{m+2,\alpha}(\Omega)$ and is equipped with the image norm

$$\|\psi\|_{W^{m+2-1/\alpha,\alpha}(\Gamma)} = \inf_{\gamma_0\mathbf{u}=\psi}\|\mathbf{u}\|_{\mathbf{W}^{m+2,\alpha}(\Omega)}.$$

Proposition 2.2.1. *Let Ω be an open set of $\mathbb{R}^N$, $N = 2$ or 3, of class C^r, $r = \max(m+2, 2)$, m integer ≥ -1, and let $\mathbf{f} \in \mathbf{W}^{m,\alpha}(\Omega)$, $f_{\text{div}} \in W^{m+1,\alpha}(\Omega)$, $\mathbf{u}_\Gamma \in \mathbf{W}^{m+2-1/\alpha,\alpha}(\Gamma)$ be given satisfying the compatibility condition*

$$\int_\Omega f_{\text{div}} \mathrm{d}\mathbf{x} = \int_\Gamma \mathbf{u}_\Gamma \cdot \mathbf{n} \mathrm{d}\Gamma.$$

Then there exist unique functions $\mathbf{u}$ and p (p is unique up to a constant) which are solutions of (S) and satisfy $\mathbf{u} \in \mathbf{W}^{m+2,\alpha}(\Omega)$, $p \in \mathbf{W}^{m+1,\alpha}(\Omega)$, and (2.2.24) with $d_\alpha = 0$ for any α, $1 < \alpha < \infty$.

2.3 Instationary Stokes equations*

In this section, we consider the following instationary Stokes equations

$$\begin{cases} \partial_t \mathbf{u} - \nu \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \mathbf{f}, & \text{in } (0,T) \times \Omega, \\ \nabla \cdot \mathbf{u} = f_{\text{div}}, & \text{in } (0,T) \times \Omega. \end{cases} \tag{iS}$$

If we set

$$P := \begin{bmatrix} -\nu\Delta & \nabla \\ \nabla\cdot & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ f_{\text{div}} \end{bmatrix},$$

then (iS) can be rewritten in the form of (gnhBVP).

Chapter 3

Shape Optimization for Incompressible Navier-Stokes Equations

3.1 Incompressible Navier-Stokes equations: Various Variants

For the derivation of Navier-Stokes equation in general and incompressible Navier-Stokes equation in particular, see, e.g., Ferziger, Perić, and Street, 2020, Moukalled, Mangani, and Darwish, 2016, Chacón Rebollo and Lewandowski, 2014.

We consider the following continuity and momentum equations of a general incompressible Navier-Stokes equations (see, e.g., Ferziger, Perić, and Street, 2020, Subsubsect. 1.7.1):

$$\begin{cases} \partial_t \mathbf{u} - \mathrm{diff}(\nu, \mathbf{u}) + \mathrm{conv}(\mathbf{u}) + \nabla p = f(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } (0,T) \times \Omega, \\ \nabla \cdot \mathbf{u} = f_{\mathrm{div}}(t, \mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } (0,T) \times \Omega. \end{cases} \tag{3.1.1}$$

$$\begin{cases} \partial_t (\rho \mathbf{u}) - \mathrm{diff}(\nu, \rho, \mathbf{u}) + \mathrm{conv}(\rho, \mathbf{u}) + \nabla p = f(\mathbf{x}, \rho, \mathbf{u}, \nabla \mathbf{u}, p), & \text{in } (0,T) \times \Omega, \\ \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, & \text{in } (0,T) \times \Omega. \end{cases} \tag{3.1.2}$$

$$\begin{cases} \partial_t \mathbf{u} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (\nu \nabla \mathbf{u}) - \dfrac{1}{\rho} \nabla p + \mathbf{b}, & \text{in } (0,T) \times \Omega, \\ \nabla \cdot \mathbf{u} = 0, & \text{in } (0,T) \times \Omega. \end{cases} \tag{3.1.3}$$

Newtonian NSEs:

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, & \text{in } (0,T) \times \Omega, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^\top) \right] + \mathbf{b}, & \text{in } (0,T) \times \Omega. \end{cases} \tag{3.1.4}$$

General NSEs:

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, & \text{in } (0,T) \times \Omega, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \boldsymbol{\tau} - \nabla p + \rho \mathbf{b}, & \text{in } (0,T) \times \Omega. \end{cases} \tag{gNSEs}$$

We recall various variants of incompressible Navier-Stokes equations in the literature (see, e.g., Chacón Rebollo and Lewandowski, 2014, Subsect. 2.6.4).

- **Basic form.**

$$\begin{cases} \partial_t \mathbf{u} - \nabla \cdot (2\nu\boldsymbol{\varepsilon}(\mathbf{u})) + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \text{in } (0,T)\times\Omega, \\ \mathbf{u}_0 = \mathbf{u}(0,\cdot), & \text{in } \Omega, \end{cases} \tag{3.1.5}$$

where the *external forcing* $\mathbf{f} : (0,T)\times\Omega \to \mathbb{R}^N$ and the *initial velocity* $\mathbf{u}_0 : \Omega \to \mathbb{R}^N$ are given.

The knowledge of the initial value of the pressure p is not required here since it is not a prognostic variable.

- **Constant viscosity case.** If we consider an *adiabatic flow* whose viscosity ν remains constant, then (3.1.5) becomes

$$\begin{cases} \partial_t \mathbf{u} - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \text{in } (0,T)\times\Omega, \\ \mathbf{u}_0 = \mathbf{u}(0,\cdot), & \text{in } \Omega, \end{cases} \tag{3.1.6}$$

- **The nonlinear term in divergence form.**

$$\begin{cases} \partial_t \mathbf{u} - \nabla \cdot (2\nu\boldsymbol{\varepsilon}(\mathbf{u})) + \nabla\cdot(\mathbf{u}\otimes\mathbf{u}) + \nabla p = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \text{on } (0,T)\times\Omega, \end{cases} \tag{3.1.7}$$

or equivalently,

$$\begin{cases} \partial_t \mathbf{u} + \nabla \cdot (-2\nu\boldsymbol{\varepsilon}(\mathbf{u}) + \mathbf{u}\otimes\mathbf{u} + p\mathbf{I}) = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \text{on } (0,T)\times\Omega, \end{cases} \tag{3.1.8}$$

which may be interesting, especially when $\mathbf{f}$ is a *restoring force*, i.e., $\mathbf{f} = \nabla\cdot\boldsymbol{\phi}$ for some vector field $\boldsymbol{\phi}$.

Remark 3.1.1. *The system* (3.1.8) *indicates that the general incompressible instationary Navier-Stokes equations can be considered as a* conservative law *of the form*

$$\begin{cases} \partial_t \mathbf{u} + \nabla\cdot P(\mathbf{u},p) = 0, & \textit{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \textit{in } (0,T)\times\Omega. \end{cases}$$

Thus standard techniques of conservation laws can be then applied to study (3.1.5)*, see, e.g., LeVeque, 2002.*

- **Form with the vorticity.**

$$\begin{cases} \partial_t \mathbf{u} - \nabla \cdot (2\nu\boldsymbol{\varepsilon}(\mathbf{u})) + \boldsymbol{\omega}\times\mathbf{u} + \nabla\left(p + \dfrac{|\mathbf{u}|^2}{2}\right) = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \text{in } (0,T)\times\Omega. \end{cases} \tag{3.1.9}$$

- **Rotating fluids.** With $\boldsymbol{\Omega}$ an *angular velocity*,

$$\begin{cases} \partial_t \mathbf{u} - \nabla \cdot (2\nu\boldsymbol{\varepsilon}(\mathbf{u})) + (\mathbf{u}\cdot\nabla)\mathbf{u} - 2\boldsymbol{\Omega}\times\mathbf{u} + \nabla p = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0, & \text{in } (0,T)\times\Omega. \end{cases} \tag{3.1.10}$$

3.2 Boundary conditions

See Chacón Rebollo and Lewandowski, 2014, Sect. 2.7 for a comprehensive list of boundary conditions which are commonly used in the literature of fluid dynamics.

We list here some possibilities of the boundary operators $(Q_i)_{1\le i\le n_{\rm bc}}$ in (gnhBVP).

- **Periodic boundary conditions.** Despite being the least physical boundary conditions, periodic boundary conditions still remain very popular due to their great advantage of using Fourier analysis to study (3.1.5), especially in the case of constant viscosity, i.e., (3.1.6).
- **The full space.** In this case, the flow domain Ω is $\mathbb{R}^3$. The following *integrability condition* is imposed:

$$\mathbf{u}(t,\cdot)\in L^2(\mathbb{R}^3)^3, \text{ for almost all } t\in\mathbb{R}_{\ge 0}.$$

- **No-slip condition.** The *no-slip condition* is of the following form

$$\mathbf{u}(t,\mathbf{x})=\mathbf{0},\ \forall(t,\mathbf{x})\in\mathbb{R}_{\ge 0}\times\Gamma, \tag{no-slipBC}$$

  or more simply $\mathbf{u}|_\Gamma=\mathbf{0}$, which is also called *homogeneous Dirichlet boundary condition* as commonly used in PDEs.

- **Navier boundary condition.** The Navier boundary condition represents a balance between slip and friction.

  Assume that Γ is not *porous*, such that no fluid particle crosses Γ, which means $\mathbf{u}=\mathbf{u}_\tau$ a.e. on Γ, or equivalently the *impermeability condition* (see, e.g., Pope, 2000, Sect. 2.4) $\mathbf{u}\cdot\mathbf{n}|_\Gamma=0$.

  The Navier boundary conditions are

$$\mathbf{u}\cdot\mathbf{n}|_\Gamma=0,\ (\mathbf{u}+\alpha(\boldsymbol{\sigma}\cdot\mathbf{n}_\tau))|_\Gamma=\mathbf{0},\ \text{for some } \alpha>0.$$

- **Wall law.**

$$\mathbf{u}\cdot\mathbf{n}|_\Gamma=0,\ (\boldsymbol{\sigma}\cdot\mathbf{n})_\tau|_\Gamma=C(\mathbf{U}_0-\mathbf{u}_\tau)|\mathbf{U}_0-\mathbf{u}_\tau|,\ \text{for some given } \mathbf{U}_0.$$

3.3 FVM for (gNSEs)*

3.3.1 Discretization of convection term*

3.3.2 Discretization of viscous term*

3.4 Domains in $\mathbb{R}^d$

We denote by $\Omega\subset\mathbb{R}^d$ an open bounded set (hence $\overline{\Omega}$ is compact). Let $\Gamma:=\partial\Omega$ denote the boundary of Ω and $\mathbf{n}$ its outer normal vector. Note that if Γ is $C^{0,1}$ then $\mathbf{n}\in L^\infty(\Gamma)$. We denote by $\mathcal{N}_0$ an unitary extension of $\mathbf{n}$, $\mathcal{N}_0$ is defined in a neighborhood of $\overline{\Omega}$ in $\mathbb{R}^d$.

3.5 NSEs

Let $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$, be an open bounded connected set. We consider the BVP for the stationary Navier-Stokes equations with mixed boundary conditions:

$$\begin{cases} (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\Delta\mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega, \\ \nabla\cdot\mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = \mathbf{f}_{\text{in}} & \text{on } \Gamma_{\text{in}}, \\ \mathbf{u} = \mathbf{0} & \text{on } \Gamma_{\text{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{u} + p\mathbf{n} = \mathbf{0} & \text{on } \Gamma_{\text{out}}. \end{cases} \tag{NSEs}$$

The velocity vector is denoted by $\mathbf{u} : \Omega \to \mathbb{R}^d$ and $p : \Omega \to \mathbb{R}$ denotes the kinematic pressure. We assume that the inflow profile $\mathbf{f}_{\text{in}} \in H^{1/2}(\Gamma_{\text{in}})^d$, the kinematic viscosity $\nu > 0$ and the density of external volume force $\mathbf{f} : \Omega \to \mathbb{R}^d$ are given.

Definition 3.5.1 (Weak solution). *A vector function* $(\mathbf{u}, p) \in W^{1,2}(\Omega)^3 \times L^2(\Omega)$ *is called a* weak solution *of* (NSEs) *if it satisfies*

$$\int_\Omega \nu\nabla\mathbf{u} : \nabla\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p\nabla\cdot\mathbf{v}\mathrm{d}x = \int_\Omega \mathbf{f}\cdot\mathbf{v}\mathrm{d}x,\ \forall\mathbf{v}\in V(\Omega), \tag{3.5.1}$$

$$\nabla\cdot\mathbf{u} = 0 \ \textit{in}\ \Omega,\ \mathbf{u}|_{\Gamma_{\text{in}}} = \mathbf{f}_{\text{in}},\ \mathbf{u}|_{\Gamma_{\text{wall}}} = \mathbf{0}, \tag{3.5.2}$$

where $V(\Omega) = \{\mathbf{v} \in W^{1,2}(\Omega)^3; \mathbf{v}|_{\Gamma_{\text{in}}\cup\Gamma_{\text{wall}}} = \mathbf{0}\}$*.*

3.6 Wellposedness of NSEs

[See Martin Kanitsar's draft/Maz'ya-Rossmann]

3.7 Cost functionals

Outflow uniformity: The uniformity of the flow upon leaving the outlet plane is an important design criterion of e.g. *automotive air ducts*. Other use: Efficiency of distributing fresh air inside the car.

$$J_1(\mathbf{u},\Omega) := \frac{1}{2}\int_{\Gamma_{\text{out}}} (\mathbf{u}\cdot\mathbf{n} - \overline{u})^2\mathrm{d}s \text{ with } \overline{u} := -\frac{1}{|\Gamma_{\text{out}}|}\int_{\Gamma_{\text{in}}} \mathbf{f}_{\text{in}}\cdot\mathbf{n}\mathrm{d}s. \tag{3.7.1}$$

Energy dissipation: Compute power dissipated by a fluid dynamic device as the net inward flux of energy.

I.e., total pressure, through the device boundaries for smooth pressure p: $\epsilon > 0$

$$J_2^\epsilon(\mathbf{u},p,\Omega) := -\frac{|\Gamma_{\text{in}}|}{|\Gamma_{\text{in}}^\epsilon|}\int_{\Gamma_{\text{in}}^\epsilon}\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x - \frac{|\Gamma_{\text{out}}|}{|\Gamma_{\text{out}}^\epsilon|}\int_{\Gamma_{\text{out}}^\epsilon}\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x = \int_\Omega k_\epsilon\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x, \tag{3.7.2}$$

where

$$k_\epsilon(x) := -\frac{|\Gamma_{\text{in}}|}{|\Gamma_{\text{in}}^\epsilon|}\chi_{\overline{\Gamma_{\text{in}}^\epsilon}}(x) - \frac{|\Gamma_{\text{out}}|}{|\Gamma_{\text{out}}^\epsilon|}\chi_{\overline{\Gamma_{\text{out}}^\epsilon}}(x),\ \forall x\in\Omega, \tag{3.7.3}$$

here χ_A denotes the characteristic function of at set A.

Note that we have used Lebesgue measure in $\mathbb{R}^d$ for $\Gamma^\epsilon_{\text{in}}, \Gamma^\epsilon_{\text{out}}$ and Lebesgue measure in $\mathbb{R}^{d-1}$ for $\Gamma_{\text{in}}, \Gamma_{\text{out}}$.

We consider the mixed cost functional with a weighting parameter $\gamma \in [0,1]$,

$$\begin{aligned} J^{\epsilon,\gamma}_{12}(\mathbf{u}, p, \Omega) &:= (1-\gamma)J_1(\mathbf{u},\Omega) + \gamma J^\epsilon_2(\mathbf{u}, p, \Omega) && (3.7.4)\\ &= \frac{1-\gamma}{2}\int_{\Gamma_{\text{out}}} (\mathbf{u}\cdot\mathbf{n} - \overline{u})^2 \mathrm{d}s + \int_\Omega \gamma k_\epsilon \left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x. && (3.7.5)\end{aligned}$$

Decomposing $J^{\epsilon,\gamma}_{12}$ into contributions from the boundary $\Gamma = \partial\Omega$ and from the interior of Ω,

$$J^{\epsilon,\gamma}_{12}(\mathbf{u}, p, \Omega) = \int_\Gamma J_\Gamma \mathrm{d}s + \int_\Omega J_\Omega \mathrm{d}x, \tag{3.7.6}$$

thus

$$\partial_{\mathbf{u}} J^{\epsilon,\gamma}_{12}(\mathbf{u}, p, \Omega)\cdot\delta\mathbf{u} = \int_\Gamma \partial_{\mathbf{u}} J_\Gamma \cdot \delta\mathbf{u}\mathrm{d}s + \int_\Omega \partial_{\mathbf{u}} J_\Omega\cdot\delta\mathbf{u}\mathrm{d}x,\ \partial_p J^{\epsilon,\gamma}_{12}\delta p = \int_\Gamma \partial_p J_\Gamma \delta p \mathrm{d}s + \int_\Omega \partial_p J_\Omega \delta p\mathrm{d}x. \tag{3.7.7}$$

We have

$$\begin{aligned} J_\Omega(\mathbf{u}, p) &= \gamma k_\epsilon \left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}, && (3.7.8)\\ \partial_{\mathbf{u}} J_\Omega(\mathbf{u}, p) &= \gamma k_\epsilon \left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right),\ \partial_p J_\Omega(\mathbf{u}, p) = \gamma k_\epsilon \mathbf{u}\cdot\mathbf{n}, && (3.7.9)\end{aligned}$$

and

$$\begin{aligned} J_\Gamma(\mathbf{u}) &= \frac{1-\gamma}{2}(\mathbf{u}\cdot\mathbf{n} - \overline{u})^2, && (3.7.10)\\ \partial_{\mathbf{u}} J_\Gamma(\mathbf{u}) &= (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n},\ \partial_p J_\Gamma(\mathbf{u}) = 0. && (3.7.11)\end{aligned}$$

3.8 Optimization problem

The optimization problems can be formulated as follows: Find Ω over a class of admissible domain $\mathcal{O}_{\text{ad}}$ such that the cost functional $J^{\epsilon,\gamma}_{12}$ is minimized subject to the NSEs (NSEs),

$$\min_{\Omega\in\mathcal{O}_{\text{ad}}} J^{\epsilon,\gamma}_{12}(\mathbf{u}, p, \Omega) \text{ such that } (\mathbf{u}, p) \text{ solves (NSEs)}. \tag{3.8.1}$$

3.9 Derive adjoint equation of NSEs - Kasumba, Kunisch version

For each weak solution $(\mathbf{u}, p)$ of (NSEs), we introduce the associated adjoint equation which is given by

$$\begin{cases} -\nu\Delta\mathbf{v} + \nabla\mathbf{u}\mathbf{v} - (\mathbf{u}\cdot\nabla)\mathbf{v} + \nabla q = \gamma k_\epsilon \left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) & \text{in } \Omega,\\ \nabla\cdot\mathbf{v} = -\gamma k_\epsilon \mathbf{u}\cdot\mathbf{n} & \text{in } \Omega,\\ \mathbf{v} = \mathbf{0} & \text{on } \Gamma_{\text{in}}\cup\Gamma_{\text{wall}},\\ -(\mathbf{u}\cdot\mathbf{n})\mathbf{v} - \nu\partial_{\mathbf{n}}\mathbf{v} + q\mathbf{n} = -(1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n} & \text{on } \Gamma_{\text{out}}. \end{cases} \tag{3.9.1}$$

Demonstration. Choose the Lagrange multiplier $(\mathbf{v}, q)$ such that the variation with respect to the state variables vanishes identically, $\partial_{\mathbf{u}}\mathcal{L} \cdot \delta\mathbf{u} + \partial_p \mathcal{L}\delta p = 0$, which reads as

$$\partial_{\mathbf{u}} J_{12}^{\epsilon,\gamma} \cdot \delta\mathbf{u} + \partial_p J_{12}^{\epsilon,\gamma}\delta p - \int_\Omega \mathbf{v}\cdot(-\nu\Delta\delta\mathbf{u} + (\delta\mathbf{u}\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)\delta\mathbf{u}) - q\nabla\cdot\delta\mathbf{u}\mathrm{d}x - \int_\Omega \mathbf{v}\cdot\nabla\delta p\mathrm{d}x$$
$$- \int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}\mathrm{d}s - \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}\mathrm{d}s - \int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot(\delta p\mathbf{n} - \nu\partial_{\mathbf{n}}\delta\mathbf{u})\mathrm{d}s = 0. \tag{3.9.2}$$

We have

$$\int_\Omega \mathbf{v}\cdot((\delta\mathbf{u}\cdot\nabla)\mathbf{u})\mathrm{d}x = \int_\Omega \mathbf{v}^\top D\mathbf{u}\delta\mathbf{u}\mathrm{d}x = \int_\Omega (\nabla\mathbf{u}\mathbf{v})\cdot\delta\mathbf{u}\mathrm{d}x.$$

We integrate by parts term by term: the second term produced by the nonlinear term $(\mathbf{u}\cdot\nabla)\mathbf{u}$:

$$\int_\Omega \mathbf{v}\cdot((\mathbf{u}\cdot\nabla)\delta\mathbf{u})\mathrm{d}x = \int_\Omega \sum_{i=1}^d\sum_{j=1}^d v_i u_j \partial_{x_j}\delta u_i \mathrm{d}x = \int_\Gamma \sum_{i=1}^d\sum_{j=1}^d v_i\delta u_i u_j n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^d\sum_{j=1}^d (\delta u_i \partial_{x_j} v_i u_j + \delta u_i v_i \partial_{x_j} u_j)\mathrm{d}x \tag{3.9.3}$$

$$= \int_\Gamma (\mathbf{u}\cdot\mathbf{n})(\mathbf{v}\cdot\delta\mathbf{u})\mathrm{d}s - \int_\Omega \left[(\mathbf{u}\cdot\nabla)\mathbf{v}\cdot\delta\mathbf{u} + \nabla\cdot\mathbf{u}(\mathbf{v}\cdot\delta\mathbf{u})\right]\mathrm{d}x = \int_\Gamma (\mathbf{u}\cdot\mathbf{n})(\mathbf{v}\cdot\delta\mathbf{u})\mathrm{d}s - \int_\Omega (\mathbf{u}\cdot\nabla) \tag{3.9.4}$$

Laplacian term:

$$-\nu\int_\Omega \mathbf{v}\cdot\Delta\delta\mathbf{u}\mathrm{d}x = -\nu\int_\Omega \sum_{i=1}^d\sum_{j=1}^d v_i\partial_{x_j}^2\delta u_i\mathrm{d}x = -\nu\int_\Gamma \sum_{i=1}^d\sum_{j=1}^d v_i\partial_{x_j}\delta u_i n_j\mathrm{d}s + \nu\int_\Omega \sum_{i=1}^d\sum_{j=1}^d \partial_{x_j}v_i\partial_{x_j}\delta u_i\mathrm{d}x \tag{3.9.5}$$

$$= -\nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \nu\int_\Gamma \sum_{i=1}^d\sum_{j=1}^d \partial_{x_j}v_i\delta u_i n_j\mathrm{d}s - \nu\int_\Omega \sum_{i=1}^d\sum_{j=1}^d \partial_{x_j}^2 v_i\delta u_i\mathrm{d}x \tag{3.9.6}$$

$$= -\nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \nu\int_\Gamma \mathbf{n}\cdot\nabla\mathbf{v}\cdot\delta\mathbf{u}\mathrm{d}s - \nu\int_\Omega \Delta\mathbf{v}\cdot\delta\mathbf{u}\mathrm{d}x, \tag{3.9.7}$$

divergence term:

$$-\int_\Omega q\nabla\cdot\delta\mathbf{u}\mathrm{d}x = \int_\Omega \delta\mathbf{u}\cdot\nabla q\mathrm{d}x - \int_\Gamma q\delta\mathbf{u}\cdot\mathbf{n}\mathrm{d}s, \tag{3.9.8}$$

and the term produced by ∇p:

$$\int_\Omega \mathbf{v}\cdot\nabla\delta p\mathrm{d}x = -\int_\Omega \delta p\nabla\cdot\mathbf{v}\mathrm{d}x + \int_\Gamma \delta p\mathbf{v}\cdot\mathbf{n}\mathrm{d}s. \tag{3.9.9}$$

We can reformulate (3.20.2) as

$$\int_\Gamma (-\mathbf{v}\cdot\mathbf{n} + \partial_p J_\Gamma)\delta p\mathrm{d}s + \int_\Omega (\nabla\cdot\mathbf{v} + \partial_p J_\Omega)\delta p\mathrm{d}x + \int_\Gamma (-(\mathbf{u}\cdot\mathbf{n})\mathbf{v} - \nu\partial_{\mathbf{n}}\mathbf{v} + q\mathbf{n} + \partial_{\mathbf{u}}J_\Gamma)\cdot\delta\mathbf{u}\mathrm{d}s$$
$$+ \nu\int_\Gamma \partial_{\mathbf{n}}\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \int_\Omega (-\nabla\mathbf{u}\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{v} + \nu\Delta\mathbf{v} - \nabla q + \partial_{\mathbf{u}}J_\Omega)\cdot\delta\mathbf{u}\mathrm{d}x$$

$$-\int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}} \cdot \delta\mathbf{u} \mathrm{d}s - \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}} \cdot \delta\mathbf{u} \mathrm{d}s - \int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}} \cdot (\delta p\mathbf{n} - \nu\partial_{\mathbf{n}}\delta\mathbf{u})\mathrm{d}s = 0. \tag{3.9.10}$$

Since this holds for any $\delta\mathbf{u}$ and δp satisfying the primal NSEs, the integrals vanish individually. The vanishing of the integrals over the domain yields the adjoint NSEs

$$\begin{cases} -\nu\Delta\mathbf{v} + \nabla\mathbf{u}\mathbf{v} - (\mathbf{u}\cdot\nabla)\mathbf{v} + \nabla q = \partial_{\mathbf{u}} J_\Omega = \gamma k_\epsilon \left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) & \text{in } \Omega, \\ \nabla\cdot\mathbf{v} = -\partial_p J_\Omega = -\gamma k_\epsilon \mathbf{u}\cdot\mathbf{n} & \text{in } \Omega. \end{cases} \tag{3.9.11}$$

As boundary conditions for adjoint velocity and pressure, deduce from (3.20.20) that

$$\int_\Gamma (-(\mathbf{u}\cdot\mathbf{n})\mathbf{v} - \nu\partial_{\mathbf{n}}\mathbf{v} + q\mathbf{n} + \partial_{\mathbf{u}} J_\Gamma)\cdot\delta\mathbf{u} + \nu\partial_{\mathbf{n}}\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s - \int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}\mathrm{d}s - \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}\mathrm{d}s + \int_{\Gamma_{\text{out}}} \nu\mathbf{v}_{\text{out}}\cdot\partial_{\mathbf{n}}\delta\mathbf{u}\mathrm{d}s \tag{3.9.12}$$

$$\int_\Gamma (-\mathbf{v}\cdot\mathbf{n} + \partial_p J_\Gamma)\delta p\mathrm{d}s - \int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot\delta p\mathbf{n}\mathrm{d}s = 0. \tag{3.9.13}$$

Since $\partial_p J_\Gamma = 0$ and $\mathbf{v} = \delta\mathbf{u} = \mathbf{0}$ on $\Gamma_{\text{in}} \cup \Gamma_{\text{wall}}$, (3.20.26) reduces to

$$\int_{\Gamma_{\text{out}}} (-\mathbf{v}\cdot\mathbf{n} - \mathbf{v}_{\text{out}}\cdot\mathbf{n})\delta p\mathrm{d}s = 0, \tag{3.9.14}$$

and thus we can set $\mathbf{v}_{\text{out}} = -\mathbf{v}$ on Γ_{out}.

Similarly, (3.20.25) reduces to

$$\int_{\Gamma_{\text{out}}} (-(\mathbf{u}\cdot\mathbf{n})\mathbf{v} - \nu\partial_{\mathbf{n}}\mathbf{v} + q\mathbf{n} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n})\cdot\delta\mathbf{u} + \nu\partial_{\mathbf{n}}\delta\mathbf{u}\cdot\mathbf{v} + \nu\mathbf{v}_{\text{out}}\cdot\partial_{\mathbf{n}}\delta\mathbf{u}\mathrm{d}s = 0. \tag{3.9.15}$$

Note that the sum of the last 2 terms vanishes, the last equation reduces to

$$\int_{\Gamma_{\text{out}}} (-(\mathbf{u}\cdot\mathbf{n})\mathbf{v} - \nu\partial_{\mathbf{n}}\mathbf{v} + q\mathbf{n} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n})\cdot\delta\mathbf{u}\mathrm{d}s = 0. \tag{3.9.16}$$

Thus,

$$-(\mathbf{u}\cdot\mathbf{n})\mathbf{v} - \nu\partial_{\mathbf{n}}\mathbf{v} + q\mathbf{n} = -(1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n} \text{ on } \Gamma_{\text{out}}. \tag{3.9.17}$$

We obtain the desired adjoint equation. □

3.10 Adjoint equation of NSEs

For each weak solution $(\mathbf{u}, p)$ of (NSEs), we introduce the associated adjoint equation which is given by

$$\begin{cases} -(\nabla\mathbf{v})^\top\cdot\mathbf{u} - \nabla\mathbf{v}\cdot\mathbf{u} - \nu\Delta\mathbf{v} + \nabla q = -\gamma k_\epsilon \left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) & \text{in } \Omega, \\ \nabla\cdot\mathbf{v} = \gamma k_\epsilon \mathbf{u}\cdot\mathbf{n} & \text{in } \Omega, \\ \mathbf{v} = \mathbf{0} & \text{on } \Gamma_{\text{in}} \cup \Gamma_{\text{wall}}, \\ (\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{n} = -(1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \bar{u})\mathbf{n} & \text{on } \Gamma_{\text{out}}, \end{cases} \tag{adjNSEs}$$

Definition 3.10.1 (Weak solution)**.** *For a given weak solution* $(\mathbf{u}, p) \in W^{1,2}(\Omega)^3 \times L^2(\Omega)$ *of* (NSEs)*, a vector function* $(\mathbf{v}, q) \in V(\Omega) \times L^2(\Omega)$ *is called a* weak solution *of* (adjNSEs) *if it satisfies*[1]

$$\int_\Omega \nu \nabla \mathbf{v} : \nabla \mathbf{w} - ((\nabla \mathbf{v})^\top \cdot \mathbf{u} + \nabla \mathbf{v} \cdot \mathbf{u}) \cdot \mathbf{w} - q \nabla \cdot \mathbf{w} dx + \int_{\Gamma_{\text{out}}} ((\mathbf{v} \cdot \mathbf{u})\mathbf{n} + (\mathbf{u} \cdot \mathbf{n})\mathbf{v} + (1-\gamma)(\mathbf{u} \cdot \mathbf{n} - \overline{u})\mathbf{n}) \cdot \mathbf{w} ds \tag{3.10.3}$$

$$= -\int_\Omega \gamma k_\epsilon \left(\left(p + \frac{1}{2}|\mathbf{u}|^2 \right) \mathbf{n} + (\mathbf{u} \cdot \mathbf{n})\mathbf{u} \right) \cdot \mathbf{w} dx, \ \forall \mathbf{w} \in V(\Omega), \tag{3.10.4}$$

$$\nabla \cdot \mathbf{v} = \gamma k_\epsilon \mathbf{u} \cdot \mathbf{n} \ \textit{in}\ \Omega, \ \mathbf{v}|_{\Gamma_{\text{in}} \cup \Gamma_{\text{wall}}} = \mathbf{0}. \tag{3.10.5}$$

3.11 Direct computation of shape derivatives without Lagrangian

From now on, let the perturbation field V belong to the following space

$$\mathcal{F}_\epsilon := \{V \in C^{1,1}(\overline{D}); V|_{\Gamma_{\text{in}}^\epsilon \cup \Gamma_{\text{out}}^\epsilon} = \mathbf{0}\}. \tag{3.11.1}$$

There exists a unique $\hat{\mathbf{f}}_{\text{in}}$ satisfying

$$\begin{cases} \nabla \cdot \hat{\mathbf{f}}_{\text{in}} = 0 & \text{in } \Omega, \\ \hat{\mathbf{f}}_{\text{in}} = \mathbf{f}_{\text{in}} & \text{on } \Gamma_{\text{in}}, \\ \hat{\mathbf{f}}_{\text{in}} = \mathbf{0} & \text{on } \Gamma_{\text{wall}} \cup \Gamma_{\text{out}}. \end{cases}$$

Let $\hat{\mathbf{u}} = \mathbf{u} - \hat{\mathbf{f}}_{\text{in}}$. Substituting $\hat{\mathbf{u}}$ into (NSEs) yields

$$\begin{cases} -\nu \Delta \hat{\mathbf{u}} + D\hat{\mathbf{u}} \cdot \hat{\mathbf{u}} + D\hat{\mathbf{u}} \cdot \hat{\mathbf{f}}_{\text{in}} + D\hat{\mathbf{f}}_{\text{in}} \cdot \hat{\mathbf{u}} + \nabla p = \mathbf{F} & \text{in } \Omega, \\ \nabla \cdot \hat{\mathbf{u}} = 0 & \text{in } \Omega, \\ \hat{\mathbf{u}} = \mathbf{0} & \text{on } \Gamma_{\text{in}} \cup \Gamma_{\text{wall}}, \\ -\nu \partial_{\mathbf{n}} \hat{\mathbf{u}} + p\mathbf{n} = \nu \partial_{\mathbf{n}} \hat{\mathbf{f}}_{\text{in}} & \text{on } \Gamma_{\text{out}}, \end{cases} \tag{3.11.2}$$

where $\mathbf{F} := \mathbf{f} + \nu \Delta \hat{\mathbf{f}}_{\text{in}} - D\hat{\mathbf{f}}_{\text{in}} \cdot \hat{\mathbf{f}}_{\text{in}}$.

Proposition 3.11.1. *We assume that the material derivative* $d\hat{\mathbf{u}}[V]$ *and* $dp[V]$ *exist. Then the shape derivatives* $\hat{\mathbf{u}}'[V] = d\hat{\mathbf{u}}[V] - D\hat{\mathbf{u}} \cdot V$ *and* $p'[V] = dp[V] - \nabla p \cdot V$ *exist by formal arguments, and they are characterized as the solution of the system*

$$\begin{cases} -\nu \Delta \hat{\mathbf{u}}'[V] + D\hat{\mathbf{u}} \cdot (\hat{\mathbf{u}}'[V] + \hat{\mathbf{g}}'[V]) + D\hat{\mathbf{u}}'[V] \cdot \mathbf{u} + D\hat{\mathbf{g}} \cdot \hat{\mathbf{u}}'[V] + D\hat{\mathbf{g}}'[V] \cdot \hat{\mathbf{u}} + \nabla p'[V] = \mathbf{F}'[V] & \textit{in } \Omega, \\ \nabla \cdot \hat{\mathbf{u}}'[V] = 0 & \textit{in } \Omega, \\ \hat{\mathbf{u}}'[V] = -V \cdot \mathbf{n} \partial_{\mathbf{n}} \hat{\mathbf{u}} & \textit{on } \Gamma_{\text{in}} \cup \Gamma_{\text{wall}} \\ -\nu \partial_{\mathbf{n}} \hat{\mathbf{u}}'[V] + p'[V]\mathbf{n} = \nu \partial_{\mathbf{n}} \hat{\mathbf{f}}'_{\text{in}}[V] & \textit{on } \Gamma_{\text{out}}, \end{cases}$$

where $\mathbf{F}'[V] = \nu \Delta \hat{\mathbf{g}}'[V] - D\hat{\mathbf{g}} \cdot \hat{\mathbf{g}}'[V] - D\hat{\mathbf{g}}'[V] \cdot \hat{\mathbf{g}}$. *Here* V *denotes a fixed deformation field.*

[1] Integrate by parts

$$-\nu \int_\Omega \Delta \mathbf{v} \cdot \mathbf{w} dx = -\nu \int_\Gamma \mathbf{n} \cdot \nabla \mathbf{v} \cdot \mathbf{w} ds + \nu \int_\Omega \nabla \mathbf{v} : \nabla \mathbf{w} dx, \tag{3.10.1}$$

$$\int_\Omega \nabla q \cdot \mathbf{w} dx = -\int_\Omega q \nabla \cdot \mathbf{w} dx + \int_\Gamma q \mathbf{w} \cdot \mathbf{n} ds. \tag{3.10.2}$$

Lemma 3.11.1. *Formally the local shape derivative* $\mathbf{u}'[V]$ *of* (NSEs) *satisfies the following system*

$$\begin{cases} -\nu\Delta\mathbf{u}'[V] + D\mathbf{u}\cdot\mathbf{u}'[V] + D\mathbf{u}'[V]\cdot\mathbf{u} + \nabla p'[V] = \mathbf{0} & \text{in } \Omega, \\ \nabla\cdot\mathbf{u}'[V] = 0 & \text{in } \Omega, \\ \mathbf{u}'[V] = -V\cdot\mathbf{n}\partial_{\mathbf{n}}(\mathbf{u}-\mathbf{f}_{\text{in}}) & \text{on } \Gamma_{\text{in}}, \\ \mathbf{u}'[V] = -V\cdot\mathbf{n}\partial_{\mathbf{n}}\mathbf{u} & \text{on } \Gamma_{\text{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{u}'[V] + p'[V]\mathbf{n} = 0 & \text{on } \Gamma_{\text{out}}. \end{cases} \tag{3.11.3}$$

Proof. * □

Lemma 3.11.2. *Formally the local shape derivative* $\mathbf{u}'[V]$ *satisfies*

$$\mathbf{u}'[V]\cdot\mathbf{n} = 0 \ \text{on } \Gamma_{\text{wall}}. \tag{3.11.4}$$

Proof. Using $\mathbf{u}'[V] = -(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}$ on Γ_{wall}, using the tangential divergence formula (1.4.22), we have on Γ_{wall} that

$$\mathbf{u}'[V]\cdot\mathbf{n} = -(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\mathbf{n} = (V\cdot\mathbf{n})\mathrm{div}_{\Gamma}\mathbf{u} - (V\cdot\mathbf{n})\nabla\cdot\mathbf{u}. \tag{3.11.5}$$

Since $\mathbf{u}|_{\Gamma_{\text{wall}}} = \mathbf{0}$, $\mathrm{div}_{\Gamma}\mathbf{u} = 0$. Combining this with $\nabla\cdot\mathbf{u} = 0$ yields the desired formula. □

Lemma 3.11.3. *The shape derivative* $dJ_{12}^{\epsilon\gamma}(\mathbf{u},p,\Omega)[V]$ *can be represented as*

(i) (Boundary representation)

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = -\int_{\Gamma_{\text{wall}}}\nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s. \tag{3.11.6}$$

(ii) (Volume representation)

Proof. (i) Applying the boundary formula for shape derivatives yields

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = \int_{\Gamma}(V\cdot\mathbf{n})\gamma k_{\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}s + \int_{\Omega}\left(\gamma k_{\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)'[V]\mathrm{d}x \tag{3.11.7}$$

$$+\frac{1-\gamma}{2}\int_{\Gamma_{\text{out}}}(V\cdot\mathbf{n})\left[\partial_{\mathbf{n}}((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)+\kappa(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2\right]+((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)'[V]\mathrm{d}s \tag{3.11.8}$$

$$= \int_{\Omega}\gamma k_{\epsilon}\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\mathbf{u}'[V]+\gamma k_{\epsilon}\mathbf{u}\cdot\mathbf{n}p'[V]\mathrm{d}x+(1-\gamma)\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u}'[V]\mathrm{d} \tag{3.11.9}$$

Testing (3.11.3) with the adjoint variable $(\mathbf{v},q)$ yields

$$\int_{\Omega}\mathbf{v}\cdot(-\nu\Delta\mathbf{u}'[V]+D\mathbf{u}\cdot\mathbf{u}'[V]+D\mathbf{u}'[V]\cdot\mathbf{u}+\nabla p'[V]) - q\nabla\cdot\mathbf{u}'[V]\mathrm{d}x = 0. \tag{3.11.10}$$

Integrating by parts (3.19.9) gives

$$\int_{\Omega}\mathbf{u}'[V]\cdot\left[-(\nabla\mathbf{v})^{\top}\cdot\mathbf{u}-\nabla\mathbf{v}\cdot\mathbf{u}-\nu\Delta\mathbf{v}+\nabla q\right]-p'[V]\nabla\cdot\mathbf{v}\mathrm{d}x \tag{3.11.11}$$

$$+\int_{\Gamma} \mathbf{u}'[V]\cdot((\mathbf{v}\cdot\mathbf{u})\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{v}+\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})-\nu\mathbf{n}\cdot\nabla\mathbf{u}'[V]\cdot\mathbf{v}+p'[V]\mathbf{v}\cdot\mathbf{n}\mathrm{d}s=0. \tag{3.11.12}$$

Since $(\mathbf{v},q)$ satisfies (adjNSEs), the last equality becomes

$$\int_{\Omega} -\mathbf{u}'[V]\cdot\gamma k_{\epsilon}\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)-\gamma k_{\epsilon}p'[V]\mathbf{u}\cdot\mathbf{n}\mathrm{d}x+\int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s \tag{3.11.13}$$

$$+\int_{\Gamma_{\text{out}}} -\mathbf{u}'[V]\cdot(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\mathrm{d}s=0. \tag{3.11.14}$$

Then (3.19.8) becomes

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V]=\int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s. \tag{3.11.15}$$

The term $\mathbf{u}'[V]\cdot q\mathbf{n}$ vanishes in Γ_{wall} due to Lemma 3.19.2. Using (3.11.3), we obtain from (3.19.14)

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V]=-\int_{\Gamma_{\text{wall}}}\nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s. \tag{3.11.16}$$

Since the mapping $V\mapsto dJ_{12}^{\epsilon\gamma}(\mathbf{u},p,\Omega)[V]V$ is linear and continuous, the shape gradient of $J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)$ is given by $\nabla J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)\mathbf{n}=-\nu(\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v})\mathbf{n}|_{\Gamma_{\text{wall}}}$.

(ii) Applying the volume formula for shape derivatives yields

$$dJ_{12}^{\epsilon\gamma}(\mathbf{u},p,\Omega)[V]=\int_{\Omega}\gamma k_{\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V+\gamma k_{\epsilon}d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]\mathrm{d}x \tag{3.11.17}$$

$$+\frac{1-\gamma}{2}\int_{\Gamma_{\text{out}}}(V\cdot\mathbf{n})\left(\partial_{\mathbf{n}}((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)+\kappa(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2\right)+((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)'[V]\mathrm{d}s \tag{3.11.18}$$

$$=\int_{\Omega}\gamma k_{\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V+\gamma k_{\epsilon}d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]\mathrm{d}x+(1-\gamma)\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u} \tag{3.11.19}$$

We compute the material derivative $d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]$ in $\Gamma_{\text{in}}^{\epsilon}\cup\Gamma_{\text{wall}}^{\epsilon}$:

$$d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]=+\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)'[V]+V\cdot\nabla\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right) \tag{3.11.20}$$

$$=\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\mathbf{u}'[V]+\mathbf{u}\cdot\mathbf{n}p'[V]+V\cdot\Big[(\nabla p+\nabla\mathbf{u}\cdot\mathbf{u})\,\mathbf{u}\cdot\mathbf{n}+\Big(p+\frac{1}{2} \tag{3.11.21}$$

Then

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V]=\int_{\Omega}\gamma k_{\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V \tag{3.11.22}$$

$$+\gamma k_{\epsilon}\left\{V\cdot\left[(\nabla p+\nabla\mathbf{u}\cdot\mathbf{u})\,\mathbf{u}\cdot\mathbf{n}+\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\nabla\mathbf{u}\cdot\mathbf{n}\right]+\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\mathbf{u}'[V]+\right. \tag{3.11.23}$$

$$+(1-\gamma)\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u}'[V]\mathrm{d}s. \tag{3.11.24}$$

We recall from (i) that

$$\int_\Omega \mathbf{u}'[V]\cdot\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)+\gamma k_\epsilon p'[V]\mathbf{u}\cdot\mathbf{n}\mathrm{d}x=\int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s+\int_{\Gamma_{\text{out}}}-\mathbf{u}'[V]\cdot(1-\gamma$$

Then

$$\begin{aligned}dJ_{12}^{\epsilon,\gamma}(\Omega)[V]=&\int_\Omega\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V+\gamma k_\epsilon V\cdot\left((\nabla p+\nabla\mathbf{u}\cdot\mathbf{u})\mathbf{u}\cdot\mathbf{n}+\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\nabla\mathbf{u}\cdot\mathbf{n}\right)\mathrm{d}x\\&+\int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s\\=&\int_\Omega\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V+\gamma k_\epsilon V\cdot\left((\nabla p+\nabla\mathbf{u}\cdot\mathbf{u})\mathbf{u}\cdot\mathbf{n}+\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\nabla\mathbf{u}\cdot\mathbf{n}\right)\mathrm{d}x\\&-\int_{\Gamma_{\text{wall}}}\nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s.\end{aligned}$$

□

Remark 3.11.1. ***Open***: *Why there are still some terms except $\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}$ left?*

3.12 Formal Lagrangian

To set up the optimality system for the shape optimization problem, we consider the following Lagrange function:

$$\begin{aligned}\mathcal{L}(\mathbf{u},p,\mathbf{v},q,\Omega,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}},\mathbf{v}_{\text{out}}):=&J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)-\int_\Omega(\mathbf{v}\cdot(-\nu\Delta\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p-\mathbf{f})-q\nabla\cdot\mathbf{u})\,\mathrm{d}x\\&-\int_{\Gamma_{\text{in}}}\mathbf{v}_{\text{in}}\cdot(\mathbf{u}-\mathbf{f}_{\text{in}})\mathrm{d}s-\int_{\Gamma_{\text{wall}}}\mathbf{v}_{\text{wall}}\cdot\mathbf{u}\mathrm{d}s-\int_{\Gamma_{\text{out}}}\mathbf{v}_{\text{out}}\cdot(p\mathbf{n}-\nu\partial_{\mathbf{n}}\mathbf{u})\mathrm{d}s,\end{aligned}\tag{3.12.1}$$

where $\mathbf{v},q,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}},\mathbf{v}_{\text{out}}$ are Lagrange multipliers.

Demonstration. Choose the Lagrange multiplier $(\mathbf{v},q)$ such that the variation with respect to the state variables vanishes identically, $\partial_{\mathbf{u}}\mathcal{L}\cdot\delta\mathbf{u}+\partial_p\mathcal{L}\delta p=0$, which reads as

$$\begin{aligned}\partial_{\mathbf{u}}J_{12}^{\epsilon,\gamma}\delta\mathbf{u}+\partial_pJ_{12}^{\epsilon,\gamma}\delta p-&\int_\Omega\mathbf{v}\cdot((\delta\mathbf{u}\cdot\nabla)\mathbf{u}+(\mathbf{u}\cdot\nabla)\delta\mathbf{u}-\nu\Delta\delta\mathbf{u})\mathrm{d}x+\int_\Omega q\nabla\cdot\delta\mathbf{u}dx-\int_\Omega\mathbf{v}\cdot\nabla\delta pdx\\&-\int_{\Gamma_{\text{in}}}\mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}ds-\int_{\Gamma_{\text{wall}}}\mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}ds-\int_{\Gamma_{\text{out}}}\mathbf{v}_{\text{out}}\cdot(\delta p\mathbf{n}-\nu\partial_{\mathbf{n}}\delta\mathbf{u})ds=0.\end{aligned}\tag{3.12.2}$$

We integrate by parts term by term: the 2 terms produced by the nonlinear term $(\mathbf{u}\cdot\nabla)\mathbf{u}$:

$$\int_\Omega\mathbf{v}\cdot((\delta\mathbf{u}\cdot\nabla)\mathbf{u})\mathrm{d}x=\int_\Omega\sum_{i=1}^d\sum_{j=1}^d v_i\partial_{x_j}u_i\delta u_j\mathrm{d}x=\int_\Gamma\sum_{i=1}^d\sum_{j=1}^d v_iu_i\delta u_jn_j\mathrm{d}s-\int_\Omega\sum_{i=1}^d\sum_{j=1}^d(u_i\partial_{x_j}v_i\delta u_j+u_iv_i\partial_{x_j}\delta u_j)\mathrm{d}x\tag{3.12.3}$$

$$=\int_\Gamma(\mathbf{v}\cdot\mathbf{u})(\delta\mathbf{u}\cdot\mathbf{n})\mathrm{d}s-\int_\Omega[\mathbf{u}\cdot\nabla\mathbf{v}^\top\cdot\delta\mathbf{u}+(\mathbf{u}\cdot\mathbf{v})\nabla\cdot\delta\mathbf{u}]\mathrm{d}x=\int_\Gamma(\mathbf{v}\cdot\mathbf{u})(\delta\mathbf{u}\cdot\mathbf{n})\mathrm{d}s-\int_\Omega\mathbf{u}\cdot\nabla\mathbf{v}^\top\tag{3.12.4}$$

$$\int_\Omega \mathbf{v}\cdot((\mathbf{u}\cdot\nabla)\delta\mathbf{u})\mathrm{d}x = \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} v_i u_j \partial_{x_j}\delta u_i \mathrm{d}x = \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d} v_i \delta u_i u_j n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} (\delta u_i \partial_{x_j} v_i u_j + \delta u_i v_i \partial_{x_j} u_j)\mathrm{d}x \tag{3.12.5}$$

$$= \int_\Gamma (\mathbf{u}\cdot\mathbf{n})(\mathbf{v}\cdot\delta\mathbf{u})\mathrm{d}s - \int_\Omega \left[(\mathbf{u}\cdot\nabla)\mathbf{v}\cdot\delta\mathbf{u} + \nabla\cdot\mathbf{u}(\mathbf{v}\cdot\delta\mathbf{u})\right]\mathrm{d}x = \int_\Gamma (\mathbf{u}\cdot\mathbf{n})(\mathbf{v}\cdot\delta\mathbf{u})\mathrm{d}s - \int_\Omega (\mathbf{u}\cdot\nabla) \tag{3.12.6}$$

Laplacian term:

$$-\nu\int_\Omega \mathbf{v}\cdot\Delta\delta\mathbf{u}\mathrm{d}x = -\nu\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} v_i \partial_{x_j}^2 \delta u_i \mathrm{d}x = -\nu\int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d} v_i \partial_{x_j}\delta u_i n_j \mathrm{d}s + \nu\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} \partial_{x_j} v_i \partial_{x_j}\delta u_i \mathrm{d}x \tag{3.12.7}$$

$$= -\nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \nu\int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d} \partial_{x_j} v_i \delta u_i n_j \mathrm{d}s - \nu\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} \partial_{x_j}^2 v_i \delta u_i \mathrm{d}x \tag{3.12.8}$$

$$= -\nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \nu\int_\Gamma \mathbf{n}\cdot\nabla\mathbf{v}\cdot\delta\mathbf{u}\mathrm{d}s - \nu\int_\Omega \Delta\mathbf{v}\cdot\delta\mathbf{u}\mathrm{d}x, \tag{3.12.9}$$

divergence term:

$$-\int_\Omega q\nabla\cdot\delta\mathbf{u}\mathrm{d}x = \int_\Omega \delta\mathbf{u}\cdot\nabla q\mathrm{d}x - \int_\Gamma q\delta\mathbf{u}\cdot\mathbf{n}\mathrm{d}s, \tag{3.12.10}$$

and the term produced by ∇p:

$$\int_\Omega \mathbf{v}\cdot\nabla\delta p\mathrm{d}x = -\int_\Omega \delta p\nabla\cdot\mathbf{v}\mathrm{d}x + \int_\Gamma \delta p\mathbf{v}\cdot\mathbf{n}\mathrm{d}s. \tag{3.12.11}$$

Decomposing $J_{12}^{\epsilon,\gamma}$ into contributions from the boundary $\Gamma = \partial\Omega$ and from the interior of Ω,

$$J_{12}^{\epsilon,\gamma} = \int_\Gamma J_\Gamma \mathrm{d}s + \int_\Omega J_\Omega \mathrm{d}x, \tag{3.12.12}$$

thus

$$\partial_{\mathbf{u}} J_{12}^{\epsilon,\gamma}\delta\mathbf{u} = \int_\Gamma \partial_{\mathbf{u}} J_\Gamma \delta\mathbf{u}\mathrm{d}s + \int_\Omega \partial_{\mathbf{u}} J_\Omega \delta\mathbf{u}\mathrm{d}x, \tag{3.12.13}$$

$$\partial_p J_{12}^{\epsilon,\gamma}\delta p = \int_\Gamma \partial_p J_\Gamma \delta p\mathrm{d}s + \int_\Omega \partial_p J_\Omega \delta p\mathrm{d}x, \tag{3.12.14}$$

we can reformulate (3.20.2) as

$$\begin{aligned}
&\int_\Gamma (\mathbf{v}\cdot\mathbf{n} - \partial_p J_\Gamma)\delta p\mathrm{d}s + \int_\Omega (-\nabla\cdot\mathbf{v} - \partial_p J_\Omega)\delta p\mathrm{d}x + \int_\Gamma \left[(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} - \partial_{\mathbf{u}} J_\Gamma\right]\cdot\delta\mathbf{u}\mathrm{d}s \\
&- \nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \int_\Omega \left[-\nabla\mathbf{v}\cdot\mathbf{u} - (\mathbf{u}\cdot\nabla)\mathbf{v} - \nu\Delta\mathbf{v} + \nabla q - \partial_{\mathbf{u}} J_\Omega\right]\cdot\delta\mathbf{u} \\
&+ \int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}ds + \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}ds + \int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot(\delta p\mathbf{n} - \nu\partial_{\mathbf{n}}\delta\mathbf{u})ds = 0.
\end{aligned} \tag{3.12.15}$$

Since this holds for any $\delta\mathbf{u}$ and δp satisfying the primal NSEs, the integrals vanish individually. The vanishing of the integrals over the domain yields the adjoint NSEs

$$\begin{cases} -2\varepsilon(\mathbf{v})\mathbf{u} = -\nabla q + \nu\Delta\mathbf{v} + \partial_{\mathbf{u}} J_\Omega & \text{in } \Omega, \\ \nabla\cdot\mathbf{v} = -\partial_p J_\Omega & \text{in } \Omega. \end{cases} \tag{3.12.16}$$

where we have expressed $-\nabla\mathbf{v}\cdot\mathbf{u} - (\mathbf{u}\cdot\nabla)\mathbf{v}$ as $-2\varepsilon(\mathbf{v})\mathbf{u}$. Then (3.20.21) becomes

$$\begin{cases} -2\varepsilon(\mathbf{v})\mathbf{u} - \nu\Delta\mathbf{v} + \nabla q = \gamma k_\epsilon \left(\left(p + \frac{1}{2}|\mathbf{u}|^2 \right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u} \right) & \text{in } \Omega, \\ \nabla\cdot\mathbf{v} = -\gamma k_\epsilon \mathbf{u}\cdot\mathbf{n} & \text{in } \Omega. \end{cases}$$

As boundary conditions for adjoint velocity and pressure, deduce from (3.20.20) that

$$\begin{aligned} &\int_\Gamma [(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} - \partial_{\mathbf{u}} J_\Gamma]\cdot\delta\mathbf{u}ds - \nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}ds \\ &\qquad + \int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}ds + \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}ds - \int_{\Gamma_{\text{out}}} \nu\mathbf{v}_{\text{out}}\cdot\partial_{\mathbf{n}}\delta\mathbf{u}ds = 0, \end{aligned} \tag{3.12.17}$$

$$\int_\Gamma (\mathbf{v}\cdot\mathbf{n} - \partial_p J_\Gamma)\delta p ds + \int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot\delta p\mathbf{n}ds = 0. \tag{3.12.18}$$

Use $\mathbf{v} = \delta\mathbf{u} = \mathbf{0}$ on $\Gamma_{\text{in}}\cup\Gamma_{\text{wall}}$, (3.20.26) reduces to

$$\int_{\Gamma_{\text{out}}} (\mathbf{v}\cdot\mathbf{n} + \mathbf{v}_{\text{out}}\cdot\mathbf{n})\delta p \mathrm{d}s = 0, \tag{3.12.19}$$

and thus we can set $\mathbf{v}_{\text{out}} = -\mathbf{v}$ on Γ_{out}.

Similarly, (3.20.25) reduces to

$$\int_{\Gamma_{\text{out}}} [(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \bar{u})\mathbf{n}]\cdot\delta\mathbf{u}ds - \nu\int_{\Gamma_{\text{out}}} \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}ds - \int_{\Gamma_{\text{out}}} \nu\mathbf{v}_{\text{out}}\cdot\partial_{\mathbf{n}}\delta\mathbf{u}ds \tag{3.12.20}$$

Note that the sum of the last 2 terms vanishes, the last equation reduces to

$$\int_{\Gamma_{\text{out}}} [(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \bar{u})\mathbf{n}]\cdot\delta\mathbf{u}\mathrm{d}s = 0. \tag{3.12.21}$$

Thus,

$$(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} = -(1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \bar{u})\mathbf{n} \text{ on } \Gamma_{\text{out}}. \tag{3.12.22}$$

We obtain the desired adjoint equation. □

Lemma 3.12.1 (Navier-Stokes shape derivative)**.** *The formal shape derivative for (NSEs) is given by*

$$dJ_{12}^{\epsilon,\gamma}(\Omega)[V] = \int_{\Gamma_{\text{wall}}} \nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s. \tag{3.12.23}$$

where $\mathbf{v}$ *is the solution of the adjoint equation.*

Proof. A formal shape differentiation of the Lagrangian (3.12.1) yields

$$d\mathcal{L}(\mathbf{u},p,\mathbf{v},q,\Omega,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}},\mathbf{v}_{\text{out}})[V] = \int_\Gamma \langle V,\mathbf{n}\rangle \left[\gamma k_\epsilon \left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n} + \mathbf{v}\cdot(-\nu\Delta\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p-\mathbf{f}) - q\nabla\cdot\mathbf{u}\right] \mathrm{d} \tag{3.12.24}$$

$$+ \int_\Omega \left[\gamma k_\epsilon \left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n} + \mathbf{v}\cdot(-\nu\Delta\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p-\mathbf{f}) - q\nabla\cdot\mathbf{u}\right]'[V]\mathrm{d} \tag{3.12.25}$$

$$+ \int_{\Gamma_{\text{out}}} \left(\frac{1-\gamma}{2}(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2 - \mathbf{v}\cdot(p\mathbf{n}-\nu\partial_{\mathbf{n}}\mathbf{u})\right)'[V]\mathrm{d}s. \tag{3.12.26}$$

Since Γ_{in} and Γ_{out} are fixed, $\mathbf{u}_{\Gamma_{\text{wall}}} = \mathbf{0}$, $V|_{\Gamma_{\text{in}}\cup\Gamma_{\text{out}}} = \mathbf{0}$ and then

$$d\mathcal{L}(\mathbf{u},p,\mathbf{v},q,\Omega,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}},\mathbf{v}_{\text{out}})[V] = \int_\Omega \left[\gamma k_\epsilon \left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n} - \mathbf{v}\cdot(-\nu\Delta\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p-\mathbf{f}) + q\nabla\cdot\mathbf{u}\right]'[V]\mathrm{d}x \tag{3.12.27}$$

$$+ \int_{\Gamma_{\text{out}}} \left(\frac{1-\gamma}{2}(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2 - \mathbf{v}\cdot(p\mathbf{n}-\nu\partial_{\mathbf{n}}\mathbf{u})\right)'[V]\mathrm{d}s = \int_\Omega I_1\mathrm{d}x + \int_{\Gamma_{\text{out}}} I_2\mathrm{d}s. \tag{3.12.28}$$

We have

$$I_1 = \left[\gamma k_\epsilon \left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n} + \mathbf{v}\cdot(-\nu\Delta\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p-\mathbf{f}) - q\nabla\cdot\mathbf{u}\right]'[V] \tag{3.12.29}$$

$$= \gamma k_\epsilon \left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\mathbf{u}'[V] + \gamma k_\epsilon p'[V]\mathbf{u}\cdot\mathbf{n} + \gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}'[V] + \mathbf{v}'[V]\cdot(-\nu\Delta\mathbf{u}+(\mathbf{u}\cdot\nabla \tag{3.12.30}$$

$$+ \mathbf{v}\cdot(-\nu\Delta\mathbf{u}'[V]+(\mathbf{u}'[V]\cdot\nabla)\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}'[V]+\nabla p'[V]) - q'[V]\nabla\cdot\mathbf{u} - q\nabla\cdot\mathbf{u}'[V] \tag{3.12.31}$$

$$= \gamma k_\epsilon \left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\mathbf{u}'[V] + \gamma k_\epsilon p'[V]\mathbf{u}\cdot\mathbf{n} + \gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}'[V] \tag{3.12.32}$$

$$+ \mathbf{v}\cdot(-\nu\Delta\mathbf{u}'[V]+(\mathbf{u}'[V]\cdot\nabla)\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}'[V]+\nabla p'[V]) - q\nabla\cdot\mathbf{u}'[V]. \tag{3.12.33}$$

Integrating by parts yields

$$\int_\Omega \mathbf{v}\cdot(-\nu\Delta\mathbf{u}'[V]+(\mathbf{u}'[V]\cdot\nabla)\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}'[V]+\nabla p'[V]) - q\nabla\cdot\mathbf{u}'[V]\mathrm{d}x \tag{3.12.34}$$

$$= \int_\Omega \mathbf{u}'[V]\cdot(-(\nabla\mathbf{v})^\top\cdot\mathbf{u} - \nabla\mathbf{v}\cdot\mathbf{u} - \nu\Delta\mathbf{v} + \nabla q) - p'[V]\nabla\cdot\mathbf{v}\mathrm{d}x \tag{3.12.35}$$

$$+ \int_\Gamma \mathbf{u}'[V]\cdot((\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{n}) - \nu\mathbf{n}\cdot\nabla\mathbf{u}'[V]\cdot\mathbf{v} + p'[V]\mathbf{v}\cdot\mathbf{n}\mathrm{d}s \tag{3.12.36}$$

$$= \int_\Omega -\mathbf{u}'[V]\cdot\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) - p'[V]\gamma k_\epsilon\mathbf{u}\cdot\mathbf{n}\mathrm{d}x \tag{3.12.37}$$

$$+ \int_\Gamma \mathbf{u}'[V]\cdot((\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{n}) - \nu\mathbf{n}\cdot\nabla\mathbf{u}'[V]\cdot\mathbf{v} + p'[V]\mathbf{v}\cdot\mathbf{n}\mathrm{d}s. \tag{3.12.38}$$

Since $\mathbf{u}'[V]=0$ in Γ_{in} and $\mathbf{v}|_{\Gamma_{\text{in}}\cup\Gamma_{\text{wall}}}=\mathbf{0}$, we have

$$\int_\Gamma \mathbf{u}'[V]\cdot((\mathbf{v}\cdot\mathbf{u})\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{v}+\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s \tag{3.12.39}$$

$$=\int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s+\int_{\Gamma_{\text{out}}}\mathbf{u}'[V]\cdot((\mathbf{v}\cdot\mathbf{u})\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{v}+\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s \tag{3.12.40}$$

$$=-\int_{\Gamma_{\text{wall}}}V\cdot\mathbf{n}(\nu\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s+\int_{\Gamma_{\text{out}}}\mathbf{u}'[V]\cdot(\gamma-1)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\mathrm{d}s. \tag{3.12.41}$$

Hence

$$\int_\Omega \mathbf{v}\cdot(-\nu\Delta\mathbf{u}'[V]+(\mathbf{u}'[V]\cdot\nabla)\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u}'[V]+\nabla p'[V])-q\nabla\cdot\mathbf{u}'[V]\mathrm{d}x \tag{3.12.42}$$

$$=\int_\Omega -\mathbf{u}'[V]\cdot\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)-p'[V]\gamma k_\epsilon\mathbf{u}\cdot\mathbf{n}\mathrm{d}x \tag{3.12.43}$$

$$+\int_{\Gamma_{\text{wall}}}V\cdot\mathbf{n}(\nu\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s+\int_{\Gamma_{\text{out}}}\mathbf{u}'[V]\cdot(\gamma-1)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\mathrm{d}s+\int_{\Gamma_{\text{out}}}-\nu\mathbf{n}\cdot\nabla\mathbf{u}'[V]\cdot\mathbf{v}+p'[V]\mathbf{v}\cdot\mathbf{n}\mathrm{d}s. \tag{3.12.44}$$

Moreover,

$$I_2=\left(\frac{1-\gamma}{2}(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2-\mathbf{v}\cdot(p\mathbf{n}-\nu\partial_{\mathbf{n}}\mathbf{u})\right)'[V] \tag{3.12.45}$$

$$=(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u}'[V]+(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{u}\cdot\mathbf{n}'[V] \tag{3.12.46}$$

$$-\mathbf{v}'[V]\cdot(p\mathbf{n}-\nu\partial_{\mathbf{n}}\mathbf{u})-\mathbf{v}\cdot(p'[V]\mathbf{n}+p\mathbf{n}'[V]-\nu\nabla\mathbf{u}'[V]\cdot\mathbf{n}-\nu\nabla\mathbf{u}\cdot\mathbf{n}'[V]) \tag{3.12.47}$$

$$=(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u}'[V]-\mathbf{v}\cdot(p'[V]\mathbf{n}-\nu\nabla\mathbf{u}'[V]\cdot\mathbf{n}), \tag{3.12.48}$$

since $\mathbf{n}'[V]=\mathbf{0}$ on Γ_{out}.

Then the shape derivative $d\mathcal{L}$ becomes

$$d\mathcal{L}(\mathbf{u},p,\mathbf{v},q,\Omega,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}},\mathbf{v}_{\text{out}})[V] \tag{3.12.49}$$

$$=\int_\Omega\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\mathbf{u}'[V]+\gamma k_\epsilon p'[V]\mathbf{u}\cdot\mathbf{n}+\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}'[V] \tag{3.12.50}$$

$$-\mathbf{u}'[V]\cdot\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)-p'[V]\gamma k_\epsilon\mathbf{u}\cdot\mathbf{n}\mathrm{d}x \tag{3.12.51}$$

$$+\int_{\Gamma_{\text{wall}}}V\cdot\mathbf{n}(\nu\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s+\int_{\Gamma_{\text{out}}}\mathbf{u}'[V]\cdot(\gamma-1)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\mathrm{d}s+\int_{\Gamma_{\text{out}}}-\nu\mathbf{n}\cdot\nabla\mathbf{u}'[V]\cdot\mathbf{v}+p'[V]\mathbf{v}\cdot\mathbf{n}\mathrm{d}s \tag{3.12.52}$$

$$+\int_{\Gamma_{\text{out}}}(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u}'[V]+(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{u}\cdot\mathbf{n}'[V] \tag{3.12.53}$$

$$-\mathbf{v}\cdot(p'[V]\mathbf{n}+p\mathbf{n}'[V]-\nu\nabla\mathbf{u}'[V]\cdot\mathbf{n}-\nu\nabla\mathbf{u}\cdot\mathbf{n}'[V])\mathrm{d}s \tag{3.12.54}$$

$$=\int_\Omega\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}'[V]\mathrm{d}x+\int_{\Gamma_{\text{wall}}}V\cdot\mathbf{n}\partial_{\mathbf{n}}\mathbf{u}\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s \tag{3.12.55}$$

$$=\int_{\Gamma_{\text{wall}}}\nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s. \tag{3.12.56}$$

□

3.13 Lagrangian in weak sense

To set up the optimality system for the shape optimization problem, we consider the following Lagrange function $\mathcal{L} : W^{1,2}(\Omega)^3 \times L^2(\Omega) \times V(\Omega) \times L^2(\Omega) \times \mathcal{O}_{\text{ad}} \times L^2(\Gamma_{\text{in}})^d \times L^2(\Gamma_{\text{wall}})^d \to \mathbb{R}$:

$$\begin{aligned}\mathcal{L}(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}}) :=& J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega) + \int_\Omega \nu \nabla \mathbf{u} : \nabla \mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p\nabla\cdot\mathbf{v} - \mathbf{f}\cdot\mathbf{v} - q\nabla\cdot\mathbf{u}\mathrm{d}x \\ &+ \int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot(\mathbf{u}-\mathbf{f}_{\text{in}})\mathrm{d}s + \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\mathbf{u}\mathrm{d}s, \end{aligned} \tag{3.13.1}$$

where $\mathbf{v}, q, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}}$ are Lagrange multipliers.

Lemma 3.13.1. *Let $(\mathbf{u}, p)$ and $(\mathbf{v}, q)$ be weak solutions of (NSEs) and (adjNSEs), respectively. Then*

(i) The first variation of $\mathcal{L}$ with respect to Lagrange multipliers is zero

$$\mathcal{L}'_{(\mathbf{v},q,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}})}(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}}, \mathbf{v}_{\text{out}})(\delta\mathbf{v}, \delta q, \delta\mathbf{v}_{\text{in}}, \delta\mathbf{v}_{\text{wall}}) = 0, \tag{3.13.2}$$

for all $(\delta\mathbf{v}, \delta q, \delta\mathbf{v}_{\text{in}}, \delta\mathbf{v}_{\text{wall}}) \in V(\Omega) \times L^2(\Omega) \times L^2(\Gamma_{\text{in}})^d \times L^2(\Gamma_{\text{wall}})^d$.

(ii) The first variation of $\mathcal{L}$ with respect to state variables is zero

$$\mathcal{L}'_{(\mathbf{u},p)}(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}})(\delta\mathbf{u}, \delta p) = 0, \tag{3.13.3}$$

for all $(\delta\mathbf{u}, \delta p) \in V(\Omega) \times L^2(\Omega)$.

(iii) Then the first total variation of $\mathcal{L}$ satisfies

$$\mathcal{L}'(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}})(\delta\mathbf{u}, \delta p, \delta\mathbf{v}, \delta q, \delta\Omega, \delta\mathbf{v}_{\text{in}}, \delta\mathbf{v}_{\text{wall}}) = \mathcal{L}_\Omega(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}})(\delta\Omega), \tag{3.13.4}$$

for all $(\delta\mathbf{u}, \delta p, \delta\mathbf{v}, \delta q, \delta\Omega, \delta\mathbf{v}_{\text{in}}, \delta\mathbf{v}_{\text{wall}}) \in V(\Omega) \times L^2(\Omega) \times V(\Omega) \times C^{1,1}(\overline{D}) \times L^2(\Omega) \times L^2(\Gamma_{\text{in}})^d \times L^2(\Gamma_{\text{wall}})^d$.

Proof. (i) We have

$$\mathcal{L}'_{\mathbf{v},q,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}}}(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}}, \mathbf{v}_{\text{out}})(\delta\mathbf{v}, \delta q, \delta\mathbf{v}_{\text{in}}, \delta\mathbf{v}_{\text{wall}}) = \int_\Omega \nu\nabla\mathbf{u} : \nabla\delta\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\delta\mathbf{v} - p\nabla\cdot\delta\mathbf{v} - \mathbf{f}\cdot\delta\mathbf{v} - \delta \tag{3.13.5}$$

$$+ \int_{\Gamma_{\text{in}}} \delta\mathbf{v}_{\text{in}}\cdot(\mathbf{u}-\mathbf{f}_{\text{in}})\mathrm{d}s + \int_{\Gamma_{\text{wall}}} \delta\mathbf{v}_{\text{wall}}\cdot\mathbf{u}\mathrm{d}s, \tag{3.13.6}$$

which is zero since $(\mathbf{u}, p)$ is a weak solution of (NSEs).

(ii) Similarly,

$$\begin{aligned}\mathcal{L}'_{\mathbf{u},p}(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}})(\delta\mathbf{u}, \delta p) =& \int_\Omega \nu\nabla\delta\mathbf{u} : \nabla\mathbf{v} + (\delta\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} + (\mathbf{u}\cdot\nabla)\delta\mathbf{u}\cdot\mathbf{v} - \delta p\nabla\cdot\mathbf{v} - q\nabla\cdot\delta\mathbf{u} \\ &+ \gamma k_\epsilon\left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\delta\mathbf{u} + \gamma k_\epsilon\mathbf{u}\cdot\mathbf{n}\delta p\mathrm{d}x\end{aligned}$$

$$+\int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}} \cdot \delta\mathbf{u} \mathrm{d}s + \int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}} \cdot \delta\mathbf{u} \mathrm{d}s + \int_{\Gamma_{\text{out}}} (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n}\cdot\delta\mathbf{u}\mathrm{d}s. \tag{3.13.7}$$

Integrating by parts

$$\int_\Omega (\delta\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v}\mathrm{d}x = \int_\Omega \sum_{i=1}^d\sum_{j=1}^d \delta u_j \partial_{x_j} u_i v_i \mathrm{d}x = \int_\Gamma \sum_{i=1}^d\sum_{j=1}^d \delta u_j u_i v_i n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^d\sum_{j=1}^d (u_i \partial_{x_j}\delta u_j v_i + u_i\delta u_j \partial_{x_j} v_i)\mathrm{d}x \tag{3.13.8}$$

$$= \int_\Gamma (\mathbf{u}\cdot\mathbf{v})(\delta\mathbf{u}\cdot\mathbf{n})\mathrm{d}s - \int_\Omega (\mathbf{u}\cdot\mathbf{v})\nabla\cdot\delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{v}^\top\cdot\delta\mathbf{u}\mathrm{d}x, \tag{3.13.9}$$

$$\int_\Omega (\mathbf{u}\cdot\nabla)\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}x = \int_\Omega \sum_{i=1}^d\sum_{j=1}^d u_j \partial_{x_j}\delta u_i v_i \mathrm{d}x = \int_\Gamma \sum_{i=1}^d\sum_{j=1}^d u_j \delta u_i v_i n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^d\sum_{j=1}^d \delta u_i \partial_{x_j} u_j v_i + \delta u_i u_j \partial_{x_j} v_i \mathrm{d}x \tag{3.13.10}$$

$$= \int_\Gamma (\delta\mathbf{u}\cdot\mathbf{v})(\mathbf{u}\cdot\mathbf{n})\mathrm{d}s - \int_\Omega (\delta\mathbf{u}\cdot\mathbf{v})\nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{v}\cdot\delta\mathbf{u}\mathrm{d}x, \tag{3.13.11}$$

and then (3.13.7) becomes

$$\mathcal{L}'_{\mathbf{u},p}(\mathbf{u},p,\mathbf{v},q,\Omega,\mathbf{v}_{\text{in}},\mathbf{v}_{\text{wall}})(\delta\mathbf{u},\delta p) \tag{3.13.12}$$

$$= \int_\Omega \nu\nabla\delta\mathbf{u} : \nabla\mathbf{v} - ((\nabla\mathbf{v})^\top\cdot\mathbf{u} + \nabla\mathbf{v}\cdot\mathbf{u})\cdot\delta\mathbf{u} - q\nabla\cdot\delta\mathbf{u} \tag{3.13.13}$$

$$+\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\delta\mathbf{u} - \delta p\nabla\cdot\mathbf{v} + \gamma k_\epsilon \mathbf{u}\cdot\mathbf{n}\delta p - (\mathbf{u}\cdot\mathbf{v})\nabla\cdot\delta\mathbf{u} - (\delta\mathbf{u}\cdot\mathbf{v})\nabla\cdot\mathbf{u}\mathrm{d}x \tag{3.13.14}$$

$$+\int_{\Gamma_{\text{out}}} (\mathbf{u}\cdot\mathbf{v})(\delta\mathbf{u}\cdot\mathbf{n}) + (\delta\mathbf{u}\cdot\mathbf{v})(\mathbf{u}\cdot\mathbf{n}) + (1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\delta\mathbf{u}\mathrm{d}s = 0, \tag{3.13.15}$$

due to (3.10.3) and $\nabla\cdot\mathbf{u} = \nabla\cdot\delta\mathbf{u} = 0$.

(iii) This follows directly from (i) and (ii). □

Lemma 3.13.2. *The shape derivative $\mathcal{L}'_\Omega(V)$ can be represented as*

(i) (Boundary representation)

(ii) (Volume representation)

Proof. (i) Using (1.4.21) and (1.4.20), we obtain

$$\mathcal{L}'_\Omega[V] = \int_{\Gamma_{\text{wall}}} V\cdot\mathbf{n}\left[\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n} + \nu\nabla\mathbf{u}:\nabla\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p\nabla\cdot\mathbf{v} - \mathbf{f}\cdot\mathbf{v} - q\nabla\cdot\mathbf{u}\right]\mathrm{d}s \tag{3.13.16}$$

$$+\int_\Omega\left[\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n} + \nu\nabla\mathbf{u}:\nabla\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p\nabla\cdot\mathbf{v} - \mathbf{f}\cdot\mathbf{v} - q\nabla\cdot\mathbf{u}\right]'[V]\mathrm{d}x \tag{3.13.17}$$

$$+\frac{1-\gamma}{2}\int_{\Gamma_{\text{out}}}((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)'[V]\mathrm{d}s. \tag{3.13.18}$$

(ii) □

3.14 Instationary NSEs

We consider the following boundary value problem for the instationary Navier-Stokes equations with mixed boundary conditions:

$$\begin{cases} \mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f} & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u} = 0 & \text{in } (0,T)\times\Omega, \\ \mathbf{u}(0,\cdot) = \mathbf{u}_0 & \text{in } \Omega, \\ \mathbf{u} = \mathbf{f}_{\text{in}} & \text{on } (0,T)\times\Gamma_{\text{in}}, \\ \mathbf{u} = \mathbf{0} & \text{on } (0,T)\times\Gamma_{\text{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{u} + p\mathbf{n} = \mathbf{0} & \text{on } (0,T)\times\Gamma_{\text{out}}, \end{cases} \tag{iNSEs}$$

with a given finite time time $T < \infty$. Here $\mathbf{u} : [0,T]\times\Omega \to \mathbb{R}^d$ and $p : [0,T]\times\Omega\to\mathbb{R}$ denote the velocity vector and the kinematic pressure, respectively. We assume that the kinematic viscosity $\nu > 0$ and the density of the external volume force $\mathbf{f} \in L^2(0,T;L^2(\Omega))$, the initial condition $\mathbf{u}_0 \in L^2(\Omega)$, the inflow profile $\mathbf{f}_{\text{in}} \in L^2(0,T;H^{1/2}(\Gamma_{\text{in}})^d)$ are given.

Let

$$V(0,T;\Omega) := H^1(0,T;L^2(\Omega)^d) \cap L^2(0,T;W^{1,2}(\Omega)^d)$$

equipped with

$$\|\mathbf{v}\|_V := \|\nabla\mathbf{v}\|_{L^2(0,T;L^2(\Omega))} + \|\mathbf{v}_t\|_{L^2(0,T;L^2(\Omega))}.$$

Definition 3.14.1 (Weak solution)**.** *A vector function* $(\mathbf{u},p) \in V(0,T;\Omega)\times L^2(0,T;L^2(\Omega))$ *is called a* weak solution *of* (iNSEs) *if it satisfies*

$$\int_0^T\int_\Omega \mathbf{u}_t\cdot\mathbf{v} + \nu\nabla\mathbf{u} : \nabla\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p\nabla\cdot\mathbf{v} - \mathbf{f}\cdot\mathbf{v}\mathrm{d}x = 0,\ \forall\mathbf{v}\in V_{\mathrm{D}}(0,T;\Omega), \tag{3.14.1}$$

$$\nabla\cdot\mathbf{u} = 0 \text{ in } [0,T]\times\Omega,\ \mathbf{u}|_{[0,T]\times\Gamma_{\text{in}}} = \mathbf{f}_{\text{in}},\ \mathbf{u}|_{[0,T]\times\Gamma_{\text{wall}}} = \mathbf{0}, \tag{3.14.2}$$

where $V_{\mathrm{D}}(0,T;\Omega) := \{\mathbf{v}\in V(0,T;\Omega); \mathbf{v}|_{[0,T]\times(\Gamma_{\text{in}}\cup\Gamma_{\text{wall}})} = \mathbf{0}\}$.

3.15 Well-posedness of instationary NSEs

[Do not know yet]

3.16 Cost functionals

We consider the following two criteria.

Outflow uniformity: The uniformity of the flow upon leaving the outlet plane is an important design criterion of e.g. *automotive air ducts*. Other use: Efficiency of distributing fresh air inside the car.

$$J_1(\mathbf{u},\Omega) := \frac{1}{2}\int_0^T\int_{\Gamma_{\text{out}}} (\mathbf{u}\cdot\mathbf{n} - \overline{u})^2\mathrm{d}s\mathrm{d}t \text{ with } \overline{u} := -\frac{1}{T|\Gamma_{\text{out}}|}\int_0^T\int_{\Gamma_{\text{in}}} \mathbf{f}_{\text{in}}\cdot\mathbf{n}\mathrm{d}s\mathrm{d}t.$$

Remark 3.16.1. *Other choices of J_1:*

$$J_1(\mathbf{u}(T),\Omega) := \frac{1}{2}\int_{\Gamma_{\text{out}}} (\mathbf{u}(T)\cdot\mathbf{n}-\overline{u})^2 \mathrm{d}s \text{ with } \overline{u}(T) := -\frac{1}{|\Gamma_{\text{out}}|}\int_{\Gamma_{\text{in}}} \mathbf{f}_{\text{in}}(T)\cdot\mathbf{n}\mathrm{d}s. \tag{3.16.1}$$

or if $\mathbf{f}_{\text{in}} \in C([0,T];L^2(\Gamma_{\text{in}})^d)$, we consider

$$J_1(\mathbf{u},\Omega) := \frac{1}{2}\int_0^T\int_{\Gamma_{\text{out}}} (\mathbf{u}\cdot\mathbf{n}-\overline{u})^2 \mathrm{d}s\mathrm{d}t \text{ with } \overline{u}(t) := -\frac{1}{|\Gamma_{\text{out}}|}\int_{\Gamma_{\text{in}}} \mathbf{f}_{\text{in}}(t)\cdot\mathbf{n}\mathrm{d}s,\ \forall t\in[0,T]. \tag{3.16.2}$$

Energy dissipation: Compute power dissipated by a fluid dynamic device as the net inward flux of energy.

I.e., total pressure, through the device boundaries for smooth pressure p: for a fixed $\epsilon > 0$, we consider

$$J_2^\epsilon(\mathbf{u},p,\Omega) := -\frac{|\Gamma_{\text{in}}|}{|\Gamma_{\text{in}}^\epsilon|}\int_0^T\int_{\Gamma_{\text{in}}^\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x\mathrm{d}t - \frac{|\Gamma_{\text{out}}|}{|\Gamma_{\text{out}}^\epsilon|}\int_0^T\int_{\Gamma_{\text{out}}^\epsilon}\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x\mathrm{d}t \tag{3.16.3}$$

$$= \int_0^T\int_\Omega k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x\mathrm{d}t, \tag{3.16.4}$$

where

$$k_\epsilon(x) := -\frac{|\Gamma_{\text{in}}|}{|\Gamma_{\text{in}}^\epsilon|}\chi_{\overline{\Gamma_{\text{in}}^\epsilon}}(x) - \frac{|\Gamma_{\text{out}}|}{|\Gamma_{\text{out}}^\epsilon|}\chi_{\overline{\Gamma_{\text{out}}^\epsilon}}(x),\ \forall x\in\Omega, \tag{3.16.5}$$

here χ_A denotes the characteristic function of at set A.

Note that we have used Lebesgue measure in $\mathbb{R}^d$ for $\Gamma_{\text{in}}^\epsilon, \Gamma_{\text{out}}^\epsilon$ and Lebesgue measure in $\mathbb{R}^{d-1}$ for $\Gamma_{\text{in}}, \Gamma_{\text{out}}$.

We consider the mixed cost functional with a weighting parameter $\gamma \in [0,1]$,

$$J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega) := (1-\gamma)J_1(\mathbf{u},\Omega) + \gamma J_2^\epsilon(\mathbf{u},p,\Omega) \tag{3.16.6}$$

$$= \frac{1-\gamma}{2}\int_0^T\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2\mathrm{d}s\mathrm{d}t + \int_0^T\int_\Omega \gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}x\mathrm{d}t. \tag{3.16.7}$$

3.17 Optimization problem

The optimization problems can be formulated as follows: Find Ω over a class of admissible domain $\mathcal{O}_{\text{ad}}$ such that the cost functional $J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)$ is minimized subject to the NSEs (iNSEs),

$$\min_{\Omega\in\mathcal{O}_{\text{ad}}} J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega) \text{ such that } (\mathbf{u},p) \text{ solves (iNSEs)}. \tag{3.17.1}$$

3.18 Adjoint equation of instationary NSEs

For each weak solution $(\mathbf{u}, p) \in V(0,T;\Omega) \times L^2(0,T;L^2(\Omega))$ of (iNSEs), we introduce the associated adjoint equation which is given by

$$\begin{cases} -\mathbf{v}_t - \nu\Delta\mathbf{v} - \nabla\mathbf{v}\cdot\mathbf{u} - (\mathbf{u}\cdot\nabla)\mathbf{v} + \nabla q = -\gamma k_\epsilon\left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{v} = \gamma k_\epsilon \mathbf{u}\cdot\mathbf{n} & \text{in } (0,T)\times\Omega, \\ \mathbf{v}(T) = \mathbf{0} & \text{in } \Omega, \\ \mathbf{v} = \mathbf{0} & \text{on } (0,T)\times(\Gamma_{\text{in}}\cup\Gamma_{\text{wall}}), \\ (\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{n} = -(1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \bar{u})\mathbf{n} & \text{on } (0,T)\times\Gamma_{\text{out}}, \end{cases} \tag{adjInsNSEs}$$

Definition 3.18.1 (Weak solution). *For a given weak solution $(\mathbf{u}, p) \in V(0,T;\Omega) \times L^2(0,T;L^2(\Omega))$ of (iNSEs), a vector function $(\mathbf{v}, q) \in V_{\mathrm{D}}(0,T;\Omega) \times L^2(0,T;L^2(\Omega))$ is called a* weak solution *of (adjNSEs) if it satisfies*[2]

$$\int_0^T\int_\Omega \mathbf{v}_t\cdot\mathbf{w} + \nu\nabla\mathbf{v} : \nabla\mathbf{w} - ((\mathbf{u}\cdot\nabla)\mathbf{v} + \nabla\mathbf{v}\cdot\mathbf{u})\cdot\mathbf{w} - q\nabla\cdot\mathbf{w}\,dx\,dt \tag{3.18.3}$$

$$+ \int_0^T\int_{\Gamma_{\text{out}}} ((\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n})\cdot\mathbf{w}\,ds\,dt \tag{3.18.4}$$

$$= -\int_0^T\int_\Omega \gamma k_\epsilon\left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\mathbf{w}\,dx\,dt, \ \forall\mathbf{w}\in V(\Omega), \tag{3.18.5}$$

$$\nabla\cdot\mathbf{v} = \gamma k_\epsilon\mathbf{u}\cdot\mathbf{n} \ \textit{in } (0,T)\times\Omega, \ \mathbf{v}|_{(0,T)\times(\Gamma_{\text{in}}\cup\Gamma_{\text{wall}})} = \mathbf{0}. \tag{3.18.6}$$

3.19 Direct computation of shape derivatives without Lagrangian

From now on, let the perturbation field V belong to the following space

$$\mathcal{F}_\epsilon := \{V \in C^{1,1}(\overline{D}); V|_{\Gamma^\epsilon_{\text{in}}\cup\Gamma^\epsilon_{\text{out}}} = \mathbf{0}\}. \tag{3.19.1}$$

Lemma 3.19.1. *Formally the local shape derivative $\mathbf{u}'[V]$ of (iNSEs) satisfies the following system*

$$\begin{cases} \mathbf{u}'_t[V] - \nu\Delta\mathbf{u}'[V] + D\mathbf{u}\cdot\mathbf{u}'[V] + D\mathbf{u}'[V]\cdot\mathbf{u} + \nabla p'[V] = \mathbf{0} & \textit{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{u}'[V] = 0 & \textit{in } \Omega, \\ \mathbf{u}'(0)[V] = \mathbf{0} & \textit{in } \Omega, \\ \mathbf{u}'[V] = -V\cdot\mathbf{n}\partial_{\mathbf{n}}(\mathbf{u} - \mathbf{f}_{\text{in}}) & \textit{on } (0,T)\times\Gamma_{\text{in}}, \\ \mathbf{u}'[V] = -V\cdot\mathbf{n}\partial_{\mathbf{n}}\mathbf{u} & \textit{on } (0,T)\times\Gamma_{\text{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{u}'[V] + p'[V]\mathbf{n} = 0 & \textit{on } (0,T)\times\Gamma_{\text{out}}. \end{cases} \tag{3.19.2}$$

[2] Integrate by parts

$$-\nu\int_\Omega \Delta\mathbf{v}\cdot\mathbf{w}\,dx = -\nu\int_\Gamma \mathbf{n}\cdot\nabla\mathbf{v}\cdot\mathbf{w}\,ds + \nu\int_\Omega \nabla\mathbf{v} : \nabla\mathbf{w}\,dx, \tag{3.18.1}$$

$$\int_\Omega \nabla q\cdot\mathbf{w}\,dx = -\int_\Omega q\nabla\cdot\mathbf{w}\,dx + \int_\Gamma q\mathbf{w}\cdot\mathbf{n}\,ds. \tag{3.18.2}$$

Proof. * □

Lemma 3.19.2. *Formally the local shape derivative* $\mathbf{u}'[V]$ *satisfies*

$$\mathbf{u}'[V]\cdot\mathbf{n} = 0 \text{ on } (0,T)\times\Gamma_{\text{wall}}. \tag{3.19.3}$$

Proof. Using $\mathbf{u}'[V] = -(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}$ on $(0,T)\times\Gamma_{\text{wall}}$, using the tangential divergence formula (1.4.22), we have on $(0,T)\times\Gamma_{\text{wall}}$ that

$$\mathbf{u}'[V]\cdot\mathbf{n} = -(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\mathbf{n} = (V\cdot\mathbf{n})\mathrm{div}_\Gamma\mathbf{u} - (V\cdot\mathbf{n})\nabla\cdot\mathbf{u}. \tag{3.19.4}$$

Since $\mathbf{u}|_{(0,T)\times\Gamma_{\text{wall}}} = \mathbf{0}$, $\mathrm{div}_\Gamma\mathbf{u} = 0$. Combining this with $\nabla\cdot\mathbf{u} = 0$ yields the desired formula. □

Lemma 3.19.3. *The shape derivative* $dJ_{12}^{\epsilon\gamma}(\mathbf{u},p,\Omega)[V]$ *can be represented as*

(i) (Boundary representation)

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = -\int_0^T\int_{\Gamma_{\text{wall}}}\nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s\mathrm{d}t. \tag{3.19.5}$$

(ii) (Volume representation)

Proof. (i) Applying the boundary formula for shape derivatives yields

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = \int_0^T\int_\Gamma(V\cdot\mathbf{n})\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\mathrm{d}s\mathrm{d}t + \int_0^T\int_\Omega\left(\gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)'[V]\mathrm{d}x\mathrm{d}t \tag{3.19.6}$$

$$+\frac{1-\gamma}{2}\int_0^T\int_{\Gamma_{\text{out}}}(V\cdot\mathbf{n})\left[\partial_{\mathbf{n}}((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)+\kappa(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2\right] + ((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)'[V]\mathrm{d}s\mathrm{d}t \tag{3.19.7}$$

$$= \int_0^T\int_\Omega\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\cdot\mathbf{u}'[V] + \gamma k_\epsilon\mathbf{u}\cdot\mathbf{n}p'[V]\mathrm{d}x\mathrm{d}t + (1-\gamma)\int_0^T\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}- \tag{3.19.8}$$

Testing (3.11.3) with the adjoint variable $(\mathbf{v},q)$ yields

$$\int_0^T\int_\Omega\mathbf{v}\cdot(\mathbf{u}_t'[V]-\nu\Delta\mathbf{u}'[V]+D\mathbf{u}\cdot\mathbf{u}'[V]+D\mathbf{u}'[V]\cdot\mathbf{u}+\nabla p'[V]) - q\nabla\cdot\mathbf{u}'[V]\mathrm{d}x\mathrm{d}t = 0. \tag{3.19.9}$$

Integrating by parts (3.19.9) gives

$$\int_0^T\int_\Omega\mathbf{u}'[V]\cdot\left[-\mathbf{v}_t-\nu\Delta\mathbf{v}-(\nabla\mathbf{v})^\top\cdot\mathbf{u}-\nabla\mathbf{v}\cdot\mathbf{u}+\nabla q\right] - p'[V]\nabla\cdot\mathbf{v}\mathrm{d}x\mathrm{d}t + \int_\Omega\mathbf{v}(T)\cdot\mathbf{u}'[V](T)-\mathbf{v}(0)\cdot\mathbf{u}'[V](0)\mathrm{d}x \tag{3.19.10}$$

$$+\int_0^T\int_\Gamma\mathbf{u}'[V]\cdot((\mathbf{v}\cdot\mathbf{u})\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{v}+\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n}) - \nu\mathbf{n}\cdot\nabla\mathbf{u}'[V]\cdot\mathbf{v}+p'[V]\mathbf{v}\cdot\mathbf{n}\mathrm{d}s\mathrm{d}t = 0. \tag{3.19.11}$$

Since $(\mathbf{v},q)$ satisfies (adjNSEs), the last equality becomes

$$\int_0^T\int_\Omega-\mathbf{u}'[V]\cdot\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) - \gamma k_\epsilon p'[V]\mathbf{u}\cdot\mathbf{n}\mathrm{d}x\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s\mathrm{d}t \tag{3.19.12}$$

$$+\int_0^T\int_{\Gamma_{\text{out}}} -\mathbf{u}'[V]\cdot(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\mathrm{d}s\mathrm{d}t = 0. \tag{3.19.13}$$

Then (3.19.8) becomes

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = \int_0^T\int_{\Gamma_{\text{wall}}} \mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s\mathrm{d}t. \tag{3.19.14}$$

The term $\mathbf{u}'[V]\cdot q\mathbf{n}$ vanishes in Γ_{wall} due to Lemma 3.19.2. Using (3.11.3), we obtain from (3.19.14)

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = -\int_0^T\int_{\Gamma_{\text{wall}}} \nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s\mathrm{d}t. \tag{3.19.15}$$

Since the mapping $V\mapsto dJ_{12}^{\epsilon\gamma}(\mathbf{u},p,\Omega)[V]V$ is linear and continuous, the shape gradient of $J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)$ is given by $\nabla J_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)\mathbf{n} = -\int_0^T \nu(\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v})\mathbf{n}|_{\Gamma_{\text{wall}}}\mathrm{d}t$.

(ii) Applying the volume formula for shape derivatives yields

$$dJ_{12}^{\epsilon\gamma}(\mathbf{u},p,\Omega)[V] = \int_\Omega \gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V + \gamma k_\epsilon d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]\mathrm{d}x \tag{3.19.16}$$

$$+\frac{1-\gamma}{2}\int_{\Gamma_{\text{out}}}(V\cdot\mathbf{n})\left(\partial_{\mathbf{n}}((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)+\kappa(\mathbf{u}\cdot\mathbf{n}-\overline{u})^2\right)+((\mathbf{u}\cdot\mathbf{n}-\overline{u})^2)'[V]\mathrm{d}s \tag{3.19.17}$$

$$= \int_\Omega \gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V + \gamma k_\epsilon d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]\mathrm{d}x + (1-\gamma)\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u} \tag{3.19.18}$$

We compute the material derivative $d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V]$ in $\Gamma_{\text{in}}^\epsilon\cup\Gamma_{\text{wall}}^\epsilon$:

$$d\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)[V] = +\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right)'[V] + V\cdot\nabla\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\right) \tag{3.19.19}$$

$$= \left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\mathbf{u}'[V]+\mathbf{u}\cdot\mathbf{n}p'[V]+V\cdot\left[(\nabla p+\nabla\mathbf{u}\cdot\mathbf{u})\,\mathbf{u}\cdot\mathbf{n}+\left(p+\frac{1}{2}\right.\right. \tag{3.19.20}$$

Then

$$dJ_{12}^{\epsilon,\gamma}(\mathbf{u},p,\Omega)[V] = \int_\Omega \gamma k_\epsilon\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}\nabla\cdot V \tag{3.19.21}$$

$$+\gamma k_\epsilon\left\{V\cdot\left[(\nabla p+\nabla\mathbf{u}\cdot\mathbf{u})\,\mathbf{u}\cdot\mathbf{n}+\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\nabla\mathbf{u}\cdot\mathbf{n}\right]+\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)\mathbf{u}'[V]+\right. \tag{3.19.22}$$

$$+(1-\gamma)\int_{\Gamma_{\text{out}}}(\mathbf{u}\cdot\mathbf{n}-\overline{u})\mathbf{n}\cdot\mathbf{u}'[V]\mathrm{d}s. \tag{3.19.23}$$

We recall from (i) that

$$\int_\Omega \mathbf{u}'[V]\cdot\gamma k_\epsilon\left(\left(p+\frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n}+(\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right)+\gamma k_\epsilon p'[V]\mathbf{u}\cdot\mathbf{n}\mathrm{d}x = \int_{\Gamma_{\text{wall}}}\mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v}-q\mathbf{n})\mathrm{d}s+\int_{\Gamma_{\text{out}}}-\mathbf{u}'[V]\cdot(1-\gamma$$

Then

$$
\begin{aligned}
dJ_{12}^{\epsilon,\gamma}(\Omega)[V] = & \int_\Omega \gamma k_\epsilon \left(p + \frac{1}{2}|\mathbf{u}|^2\right) \mathbf{u}\cdot\mathbf{n}\nabla\cdot V + \gamma k_\epsilon V \cdot \left((\nabla p + \nabla\mathbf{u}\cdot\mathbf{u})\mathbf{u}\cdot\mathbf{n} + \left(p + \frac{1}{2}|\mathbf{u}|^2\right)\nabla\mathbf{u}\cdot\mathbf{n}\right) \mathrm{d}x \\
& + \int_{\Gamma_{\text{wall}}} \mathbf{u}'[V]\cdot(\nu\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{n})\mathrm{d}s \\
= & \int_\Omega \gamma k_\epsilon \left(p + \frac{1}{2}|\mathbf{u}|^2\right) \mathbf{u}\cdot\mathbf{n}\nabla\cdot V + \gamma k_\epsilon V \cdot \left((\nabla p + \nabla\mathbf{u}\cdot\mathbf{u})\mathbf{u}\cdot\mathbf{n} + \left(p + \frac{1}{2}|\mathbf{u}|^2\right)\nabla\mathbf{u}\cdot\mathbf{n}\right) \mathrm{d}x \\
& - \int_{\Gamma_{\text{wall}}} \nu(V\cdot\mathbf{n})\partial_{\mathbf{n}}\mathbf{u}\cdot\partial_{\mathbf{n}}\mathbf{v}\mathrm{d}s.
\end{aligned}
$$

□

3.20 Formal Lagrangian

To set up the optimality system for the shape optimization problem, we consider the following Lagrange function:

$$
\begin{aligned}
&\mathcal{L}(\mathbf{u}, p, \mathbf{v}, q, \Omega, \mathbf{v}_0, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}}, \mathbf{v}_{\text{out}}) := J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega) + \int_0^T \int_\Omega \mathbf{v}\cdot(\mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \mathbf{f}) - q\nabla\cdot\mathbf{u}\mathrm{d}x\mathrm{d}t \\
&+ \int_\Omega \mathbf{v}_0\cdot(\mathbf{u}(0) - \mathbf{u}_0)\mathrm{d}x + \int_0^T\int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot(\mathbf{u} - \mathbf{f}_{\text{in}})\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\mathbf{u}\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot(p\mathbf{n} - \nu\partial_{\mathbf{n}}\mathbf{u})\mathrm{d}s\mathrm{d}t,
\end{aligned}
\tag{3.20.1}
$$

where $\mathbf{v}, q, \mathbf{v}_0, \mathbf{v}_{\text{in}}, \mathbf{v}_{\text{wall}}, \mathbf{v}_{\text{out}}$ are Lagrange multipliers.

Demonstration. Choose the Lagrange multiplier $(\mathbf{v}, q)$ such that the variation with respect to the state variables vanishes identically, $\partial_{\mathbf{u}}\mathcal{L}\cdot\delta\mathbf{u} + \partial_p\mathcal{L}\delta p = 0$, which reads as

$$
\begin{aligned}
&\partial_{\mathbf{u}} J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega)\cdot\delta\mathbf{u} + \partial_p J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega)\delta p + \int_0^T\int_\Omega \mathbf{v}\cdot[\delta\mathbf{u}_t - \nu\Delta\delta\mathbf{u} + (\delta\mathbf{u}\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)\delta\mathbf{u}] - q\nabla\cdot\delta\mathbf{u} + \mathbf{v}\cdot\nabla\delta p\mathrm{d}x \\
&+ \int_\Omega \mathbf{v}_0\cdot\delta\mathbf{u}(0)\mathrm{d}x + \int_0^T\int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot(\delta p\mathbf{n} - \nu\partial_{\mathbf{n}}\delta\mathbf{u})\mathrm{d}s\mathrm{d}t = 0.
\end{aligned}
\tag{3.20.2}
$$

We integrate by parts term by term: the term involving time derivative:

$$
\int_0^T\int_\Omega \mathbf{v}\cdot\delta\mathbf{u}_t\mathrm{d}x\mathrm{d}t = \int_\Omega \mathbf{v}(T)\cdot\delta\mathbf{u}(T) - \mathbf{v}(0)\cdot\delta\mathbf{u}(0)\mathrm{d}x - \int_0^T\int_\Omega \mathbf{v}_t\cdot\delta\mathbf{u}\mathrm{d}x\mathrm{d}t, \tag{3.20.3}
$$

Laplacian term:

$$
-\nu\int_\Omega \mathbf{v}\cdot\Delta\delta\mathbf{u}\mathrm{d}x = -\nu\int_\Omega\sum_{i=1}^d\sum_{j=1}^d v_i\partial_{x_j}^2\delta u_i\mathrm{d}x = -\nu\int_\Gamma\sum_{i=1}^d\sum_{j=1}^d v_i\partial_{x_j}\delta u_i n_j\mathrm{d}s + \nu\int_\Omega\sum_{i=1}^d\sum_{j=1}^d \partial_{x_j}v_i\partial_{x_j}\delta u_i\mathrm{d}x \tag{3.20.4}
$$

$$
= -\nu\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s + \nu\int_\Gamma\sum_{i=1}^d\sum_{j=1}^d \partial_{x_j}v_i\delta u_i n_j\mathrm{d}s - \nu\int_\Omega\sum_{i=1}^d\sum_{j=1}^d \partial_{x_j}^2 v_i\delta u_i\mathrm{d}x \tag{3.20.5}
$$

$$= -\nu \int_\Gamma \mathbf{n} \cdot \nabla \delta \mathbf{u} \cdot \mathbf{v} \mathrm{d}s + \nu \int_\Gamma \mathbf{n} \cdot \nabla \mathbf{v} \cdot \delta \mathbf{u} \mathrm{d}s - \nu \int_\Omega \Delta \mathbf{v} \cdot \delta \mathbf{u} \mathrm{d}x, \tag{3.20.6}$$

the 2 terms produced by the nonlinear term $(\mathbf{u} \cdot \nabla)\mathbf{u}$:

$$\int_\Omega \mathbf{v} \cdot ((\delta \mathbf{u} \cdot \nabla)\mathbf{u}) \mathrm{d}x = \int_\Omega \sum_{i=1}^d \sum_{j=1}^d v_i \partial_{x_j} u_i \delta u_j \mathrm{d}x = \int_\Gamma \sum_{i=1}^d \sum_{j=1}^d v_i u_i \delta u_j n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^d \sum_{j=1}^d (u_i \partial_{x_j} v_i \delta u_j + u_i v_i \partial_{x_j} \delta u_j) \mathrm{d}x \tag{3.20.7}$$

$$= \int_\Gamma (\mathbf{v} \cdot \mathbf{u})(\delta \mathbf{u} \cdot \mathbf{n}) \mathrm{d}s - \int_\Omega [\mathbf{u} \cdot \nabla \mathbf{v}^\top \cdot \delta \mathbf{u} + (\mathbf{u} \cdot \mathbf{v}) \nabla \cdot \delta \mathbf{u}] \mathrm{d}x = \int_\Gamma (\mathbf{v} \cdot \mathbf{u})(\delta \mathbf{u} \cdot \mathbf{n}) \mathrm{d}s - \int_\Omega \mathbf{u} \cdot \nabla \mathbf{v}^\top \tag{3.20.8}$$

$$\int_\Omega \mathbf{v} \cdot ((\mathbf{u} \cdot \nabla)\delta \mathbf{u}) \mathrm{d}x = \int_\Omega \sum_{i=1}^d \sum_{j=1}^d v_i u_j \partial_{x_j} \delta u_i \mathrm{d}x = \int_\Gamma \sum_{i=1}^d \sum_{j=1}^d v_i \delta u_i u_j n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^d \sum_{j=1}^d (\delta u_i \partial_{x_j} v_i u_j + \delta u_i v_i \partial_{x_j} u_j) \mathrm{d}x \tag{3.20.9}$$

$$= \int_\Gamma (\mathbf{u} \cdot \mathbf{n})(\mathbf{v} \cdot \delta \mathbf{u}) \mathrm{d}s - \int_\Omega \left[(\mathbf{u} \cdot \nabla)\mathbf{v} \cdot \delta \mathbf{u} + \nabla \cdot \mathbf{u}(\mathbf{v} \cdot \delta \mathbf{u}) \right] \mathrm{d}x = \int_\Gamma (\mathbf{u} \cdot \mathbf{n})(\mathbf{v} \cdot \delta \mathbf{u}) \mathrm{d}s - \int_\Omega (\mathbf{u} \cdot \nabla) \tag{3.20.10}$$

divergence term:

$$- \int_\Omega q \nabla \cdot \delta \mathbf{u} \mathrm{d}x = \int_\Omega \delta \mathbf{u} \cdot \nabla q \mathrm{d}x - \int_\Gamma q \delta \mathbf{u} \cdot \mathbf{n} \mathrm{d}s, \tag{3.20.11}$$

and the term produced by ∇p:

$$\int_\Omega \mathbf{v} \cdot \nabla \delta p \mathrm{d}x = - \int_\Omega \delta p \nabla \cdot \mathbf{v} \mathrm{d}x + \int_\Gamma \delta p \mathbf{v} \cdot \mathbf{n} \mathrm{d}s. \tag{3.20.12}$$

Decomposing $J_{12}^{\epsilon,\gamma}$ into contributions from the boundary $\Gamma = \partial\Omega$ and from the interior of Ω,

$$J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega) = \int_0^T \int_\Gamma J_\Gamma \mathrm{d}s \mathrm{d}t + \int_0^T \int_\Omega J_\Omega \mathrm{d}x \mathrm{d}t, \tag{3.20.13}$$

thus

$$\partial_{\mathbf{u}} J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega) \cdot \delta \mathbf{u} = \int_0^T \int_\Gamma \partial_{\mathbf{u}} J_\Gamma \cdot \delta \mathbf{u} \mathrm{d}s \mathrm{d}t + \int_0^T \int_\Omega \partial_{\mathbf{u}} J_\Omega \cdot \delta \mathbf{u} \mathrm{d}x \mathrm{d}t, \tag{3.20.14}$$

$$\partial_p J_{12}^{\epsilon,\gamma}(\mathbf{u}, p, \Omega) \cdot \delta p = \int_0^T \int_\Gamma \partial_p J_\Gamma \cdot \delta p \mathrm{d}s \mathrm{d}t + \int_0^T \int_\Omega \partial_p J_\Omega \cdot \delta p \mathrm{d}x \mathrm{d}t, \tag{3.20.15}$$

we can reformulate (3.20.2) as

$$\int_0^T \int_\Gamma (\mathbf{v} \cdot \mathbf{n} + \partial_p J_\Gamma) \delta p \mathrm{d}s \mathrm{d}t + \int_0^T \int_\Omega (-\nabla \cdot \mathbf{v} + \partial_p J_\Omega) \delta p \mathrm{d}x \mathrm{d}t \tag{3.20.16}$$

$$+ \int_0^T \int_\Gamma [(\mathbf{v} \cdot \mathbf{u})\mathbf{n} + (\mathbf{u} \cdot \mathbf{n})\mathbf{v} + \nu \mathbf{n} \cdot \nabla \mathbf{v} - q\mathbf{n} + \partial_{\mathbf{u}} J_\Gamma] \cdot \delta \mathbf{u} \mathrm{d}s \mathrm{d}t \tag{3.20.17}$$

$$+ \int_0^T \int_\Omega [-\mathbf{v}_t - \nu \Delta \mathbf{v} - \nabla \mathbf{v} \cdot \mathbf{u} - (\mathbf{u} \cdot \nabla)\mathbf{v} + \nabla q + \partial_{\mathbf{u}} J_\Omega] \cdot \delta \mathbf{u} \mathrm{d}x \mathrm{d}t \tag{3.20.18}$$

$$-\int_0^T\int_\Gamma \nu \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s\mathrm{d}t + \int_\Omega \mathbf{v}(T)\cdot\delta\mathbf{u}(T) - \mathbf{v}(0)\cdot\delta\mathbf{u}(0) + \mathbf{v}_0\cdot\delta\mathbf{u}(0)\mathrm{d}x \tag{3.20.19}$$

$$+\int_0^T\int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot(\delta p\mathbf{n} - \nu\partial_{\mathbf{n}}\delta\mathbf{u})\mathrm{d}s\mathrm{d}t = 0. \tag{3.20.20}$$

Since this holds for any $\delta\mathbf{u}$ and δp satisfying the primal NSEs, the integrals vanish individually. The vanishing of the integrals over the domain yields the adjoint NSEs (choose $\delta\mathbf{u}$ s.t. $\delta\mathbf{u}(0) = \delta\mathbf{u}(T) = \mathbf{0}$)

$$\begin{cases} -\mathbf{v}_t - \nu\Delta\mathbf{v} - \nabla\mathbf{v}\cdot\mathbf{u} - (\mathbf{u}\cdot\nabla)\mathbf{v} + \nabla q = -\partial_{\mathbf{u}}J_\Omega & \text{in } \Omega, \\ \nabla\cdot\mathbf{v} = \partial_p J_\Omega & \text{in } \Omega. \end{cases} \tag{3.20.21}$$

Plugging explicit formulas of J_Ω yields

$$J_\Omega(\mathbf{u},p) = \gamma k_\epsilon\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{u}\cdot\mathbf{n}, \tag{3.20.22}$$

$$\partial_{\mathbf{u}}J_\Omega(\mathbf{u},p) = \gamma k_\epsilon\left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right), \tag{3.20.23}$$

$$\partial_p J_\Omega(\mathbf{u},p) = \gamma k_\epsilon \mathbf{u}\cdot\mathbf{n}. \tag{3.20.24}$$

Then (3.20.21) becomes

$$\begin{cases} -\mathbf{v}_t - \nu\Delta\mathbf{v} - \nabla\mathbf{v}\cdot\mathbf{u} - (\mathbf{u}\cdot\nabla)\mathbf{v} + \nabla q = -\gamma k_\epsilon\left(\left(p + \frac{1}{2}|\mathbf{u}|^2\right)\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{u}\right) & \text{in } [0,T]\times\Omega, \\ \nabla\cdot\mathbf{v} = \gamma k_\epsilon \mathbf{u}\cdot\mathbf{n} & \text{in } [0,T]\times\Omega. \end{cases}$$

The remaining terms yields

$$\int_0^T\int_\Gamma [(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} + \partial_{\mathbf{u}}J_\Gamma]\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t - \nu\int_0^T\int_\Gamma \mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}s\mathrm{d}t$$
$$+\int_0^T\int_{\Gamma_{\text{in}}} \mathbf{v}_{\text{in}}\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{wall}}} \mathbf{v}_{\text{wall}}\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t - \int_0^T\int_{\Gamma_{\text{out}}} \nu\mathbf{v}_{\text{out}}\cdot\partial_{\mathbf{n}}\delta\mathbf{u}\mathrm{d}s\mathrm{d}t = 0, \tag{3.20.25}$$

$$\int_0^T\int_\Gamma (\mathbf{v}\cdot\mathbf{n} + \partial_p J_\Gamma)\delta p\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma_{\text{out}}} \mathbf{v}_{\text{out}}\cdot\delta p\mathbf{n}\mathrm{d}s\mathrm{d}t = 0, \tag{3.20.26}$$

$$\int_\Omega \mathbf{v}(T)\cdot\delta\mathbf{u}(T) - \mathbf{v}(0)\cdot\delta\mathbf{u}(0) + \mathbf{v}_0\cdot\delta\mathbf{u}(0)\mathrm{d}x = 0. \tag{3.20.27}$$

In (3.20.27), choosing $\delta\mathbf{u}$ s.t. $\delta\mathbf{u}(0) = \mathbf{0}$ yields $\mathbf{v}(T) = 0$, and $\mathbf{v}_0 = \mathbf{v}(0)$. Plugging the explicit formula for $J_\Gamma(\mathbf{u})$ gives

$$J_\Gamma(\mathbf{u}) = \frac{1-\gamma}{2}(\mathbf{u}\cdot\mathbf{n} - \overline{u})^2, \tag{3.20.28}$$

$$\partial_{\mathbf{u}}J_\Gamma(\mathbf{u}) = (1-\gamma)(\mathbf{u}\cdot\mathbf{n} - \overline{u})\mathbf{n}, \tag{3.20.29}$$

$$\partial_p J_\Gamma(\mathbf{u}) = 0. \tag{3.20.30}$$

Use $\mathbf{v} = \delta\mathbf{u} = \mathbf{0}$ on $\Gamma_{\text{in}}\cup\Gamma_{\text{wall}}$, (3.20.26) reduces to

$$\int_0^T\int_{\Gamma_{\text{out}}} (\mathbf{v}\cdot\mathbf{n} + \mathbf{v}_{\text{out}}\cdot\mathbf{n})\delta p\mathrm{d}s\mathrm{d}t = 0, \tag{3.20.31}$$

and thus we can set $\mathbf{v}_{\rm out} = -\mathbf{v}$ on $\Gamma_{\rm out}$.

Similarly, (3.20.25) reduces to

$$\int_0^T \int_{\Gamma_{\rm out}} [(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\bar{u})\mathbf{n}]\cdot\delta\mathbf{u} - \nu\mathbf{n}\cdot\nabla\delta\mathbf{u}\cdot\mathbf{v} - \nu\mathbf{v}_{\rm out}\cdot\partial_{\mathbf{n}}\delta\mathbf{u}\mathrm{d}s\mathrm{d}t = 0. \tag{3.20.32}$$

Note that the sum of the last 2 terms vanishes, the last equation reduces to

$$\int_0^T \int_{\Gamma_{\rm out}} [(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} + (1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\bar{u})\mathbf{n}]\cdot\delta\mathbf{u}\mathrm{d}s\mathrm{d}t = 0. \tag{3.20.33}$$

Thus,

$$(\mathbf{v}\cdot\mathbf{u})\mathbf{n} + (\mathbf{u}\cdot\mathbf{n})\mathbf{v} + \nu\mathbf{n}\cdot\nabla\mathbf{v} - q\mathbf{n} = -(1-\gamma)(\mathbf{u}\cdot\mathbf{n}-\bar{u})\mathbf{n} \text{ on } [0,T]\times\Gamma_{\rm out}. \tag{3.20.34}$$

We obtain the desired adjoint equation. □

3.21 A general framework

General Outline. In this part: consider a PDEs/mathematical models (e.g., Navier-Stokes equations, Smagorinsky turbulence models, k-ϵ turbulence models, etc.) with the following outline:

1. A PDEs/mathematical models
2. Weak formulation of the considered PDEs/mathematical models
3. Adjoint equations of the considered PDEs/mathematical models
4. Weak formulation of the adjoint equations of the considered PDEs/mathematical models
5. Shape derivatives for the considered PDEs/mathematical models (with boundary conditions plugged in and other add-ons, e.g., wall laws)
   (a) 1st-order shape derivatives for the considered PDEs/mathematical models
   (b) 2nd-order shape derivatives for the considered PDEs/mathematical models [hard, added later]
6. Shape optimization for the considered PDEs/mathematical models

In this chapter, we will design a framework for shape optimization for the PDEs of the following form (with assumption that the density $\rho = \text{const}$):

$$\begin{cases} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) = \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) & \text{in } \Omega,\\ -\nabla\cdot\mathbf{u} = f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) & \text{in } \Omega,\\ \mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\rm bc}(\mathbf{x}) & \text{on } \Gamma, \end{cases} \tag{gfld}$$

where $\mathbf{P}(\cdot,\ldots,\cdot) = (P_1,\ldots,P_N)(\cdot,\ldots,\cdot)$, $\mathbf{f}(\cdot,\ldots,\cdot) = (f_1,\ldots,f_N)(\cdot,\ldots,\cdot)$ and $\mathbf{Q}(\cdot,\ldots,\cdot)$ denote the main PDE (e.g., here, NSEs), the source terms, and the set of boundary conditions, respectively.

3.21.1 Weak formulation of (gfld)

Test both sides of the 1st equation of (gfld) with a test function $\mathbf{v}$ and those of the 2nd one with a test function q over Ω:

$$\begin{cases} \displaystyle\int_\Omega \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v}\mathrm{d}\mathbf{x}, \\ \displaystyle -\int_\Omega q\nabla\cdot\mathbf{u}\mathrm{d}\mathbf{x} = \int_\Omega q f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x}, \end{cases} \tag{wf-gfld}$$

and then integrate by parts all the 2nd-order terms w.r.t. $\mathbf{u}$ and all the 1st-order terms w.r.t. p in the 1st equation of (wf-gfld).

Plugging the boundary conditions (i.e., the 3rd equation of (gfld)) into the equations just obtained to embed them into the weak formulation.

3.21.2 Cost functionals

A general cost functional for (gfld) is given by

$$J(\mathbf{u},p,\Omega) \coloneqq \int_\Omega J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x} + \int_\Gamma J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathrm{d}\Gamma. \tag{cost-gfld}$$

3.21.3 Lagrangian & extended Lagrangian

To derive the adjoint equations for (gfld), 1st introduce the following Lagrangian (see, e.g., Tröltzsch, 2010):

$$L(\mathbf{u},p,\Omega,\mathbf{v},q) \coloneqq J(\mathbf{u},p,\Omega) + \int_\Omega -\left(\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\cdot\mathbf{v} + q\left(\nabla\cdot\mathbf{u} + f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x}, \tag{L-gfld}$$

and the following extended Lagrangian:

$$\begin{aligned} \mathcal{L}(\mathbf{u},p,\Omega,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}}) &\coloneqq L(\mathbf{u},p,\Omega,\mathbf{v},q) - \int_\Gamma \left(\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{f}_{\mathrm{bc}}(\mathbf{x})\right)\cdot\mathbf{v}_{\mathrm{bc}}\mathrm{d}\Gamma \\ &= J(\mathbf{u},p,\Omega) + \int_\Omega -\left(\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\cdot\mathbf{v} + q\left(\nabla\cdot\mathbf{u} + f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x} \\ &\quad - \int_\Gamma \left(\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{f}_{\mathrm{bc}}(\mathbf{x})\right)\cdot\mathbf{v}_{\mathrm{bc}}\mathrm{d}\Gamma, \end{aligned} \tag{$\mathcal{L}$-gfld}$$

where $\mathbf{v}$, q, $\mathbf{v}_{\mathrm{bc}}$ are Lagrange multipliers.

3.21.4 Shape optimization problems

Here are 3 different shape optimization problems associated with (cost-gfld), (L-gfld), and ($\mathcal{L}$-gfld), respectively:

$$\begin{aligned} &\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} J(\mathbf{u},p,\Omega) \text{ s.t. } (\mathbf{u},p) \text{ solves (gfld)}, \\ &\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} L(\mathbf{u},p,\Omega,\mathbf{v},q) \text{ s.t. } (\mathbf{u},p) \text{ satisfies } \mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x}) \text{ on } \Gamma, \\ &\min_{\Omega\in\mathcal{O}_{\mathrm{ad}}} \mathcal{L}(\mathbf{u},p,\Omega,\mathbf{v},q,\mathbf{v}_{\mathrm{bc}}) \text{ with } (\mathbf{u},p) \text{ unconstrained.} \end{aligned}$$

In the 2nd optimization problem, the main PDEs (i.e., equations in Ω) are already penalized by implicitly embedded into the Lagrangian (L-gfld), meanwhile in the 3rd one, both main PDEs and boundary conditions are penalized by implicitly embedded into the extended Lagrangian ($\mathcal{L}$-gfld).

Remark 3.21.1. *Remind that this is just a formal framework. For a rigorous one, the correct function spaces of both state and adjoint variables need inserting into these optimization problems.*

Here $(\mathbf{u}, p)$, $(\mathbf{v}, q)$ (also $\mathbf{v}_{\rm bc}$ for the last shape optimization problem with the extended Lagrangian), and Ω are the *state variables, adjoint variables*, and *control variable* for these shape optimization problems.

3.21.5 Adjoint equations of (gfld)

A natural question arises:

Question 3.21.1. *Should the Lagrangian or the extended Lagrangian be used to derive the adjoint equations?*

To answer this question, introduce the following "mixed" Lagrangian:

$$\begin{aligned} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) &:= L(\mathbf{u}, p, \Omega, \mathbf{v}, q) - \delta_{\mathcal{L}} \int_\Gamma (\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\rm bc}(\mathbf{x})) \cdot \mathbf{v}_{\rm bc} {\rm d}\Gamma \qquad (L_{\mathcal{L}}\text{-gfld}) \\ &= J(\mathbf{u}, p, \Omega) + \int_\Omega - (\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) - \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \cdot \mathbf{v} + q\, (\nabla \cdot \mathbf{u} + f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \\ &\quad - \delta_{\mathcal{L}} \int_\Gamma (\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\rm bc}(\mathbf{x})) \cdot \mathbf{v}_{\rm bc} {\rm d}\Gamma, \text{ where } \delta_{\mathcal{L}} \in \{0, 1\}. \end{aligned}$$

Remark 3.21.2. *No need to assume the "switch" between Lagrangian and extended Lagrangian is a real number, i.e.* $\delta_{\mathcal{L}} \in \mathbb{R}$, *since the scaling is already embedded in the Lagrange multiplier* $\mathbf{v}_{\rm bc}$.

Hence,

$$L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) = \begin{cases} L(\mathbf{u}, p, \Omega, \mathbf{v}, q) & \text{if } \delta_{\mathcal{L}} = 0, \\ \mathcal{L}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) & \text{if } \delta_{\mathcal{L}} = 1. \end{cases}$$

Then the shape optimization problem reads

$$\min_{\Omega \in \mathcal{O}_{\rm ad}} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) \begin{cases} \text{s.t. } (\mathbf{u}, p) \text{ satisfies } \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\rm bc}(\mathbf{x}) \text{ on } \Gamma & \text{if } \delta_{\mathcal{L}} = 0, \\ \text{with } (\mathbf{u}, p) \text{ unconstrained} & \text{if } \delta_{\mathcal{L}} = 1. \end{cases}$$

Next, choose the Lagrangian multiplier $(\mathbf{v}, q, \mathbf{v}_{\rm bc})$ s.t. the variation of the chosen Lagrangian (simple/extended/mixed) w.r.t. state variables vanishes, i.e.:

$$\delta_{(\mathbf{u},p)} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}; \tilde{\mathbf{u}}, \tilde{p}) = 0, \ \forall (\tilde{\mathbf{u}}, \tilde{p}),$$

where

$$\begin{aligned} &\delta_{(\mathbf{u},p)} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}; \tilde{\mathbf{u}}, \tilde{p}) \\ &:= \lim_{t \downarrow 0} \frac{1}{t} (L_{\mathcal{L}}(\mathbf{u} + t\tilde{\mathbf{u}}, p + t\tilde{p}, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) - L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})) \\ &= \lim_{t \downarrow 0} \frac{1}{t} (L_{\mathcal{L}}(\mathbf{u} + t\tilde{\mathbf{u}}, p + t\tilde{p}, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) - L_{\mathcal{L}}(\mathbf{u}, p + t\tilde{p}, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})) + \lim_{t \downarrow 0} \frac{1}{t} (L_{\mathcal{L}}(\mathbf{u}, p + t\tilde{p}, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}) - L_{\mathcal{L}}(\mathbf{u}, p, \Omega \end{aligned}$$

$$= \lim_{t\downarrow 0} \delta_{\mathbf{u}} L_{\mathcal{L}}(\mathbf{u}, p + t\tilde{p}, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}; \tilde{\mathbf{u}}) + \delta_p L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}; \tilde{p}) = \delta_{\mathbf{u}} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc}; \tilde{\mathbf{u}}) + \delta_p L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm b}$$

Provided Gateaux/Fréchet differentiability of $L_{\mathcal{L}}$ is guaranteed, in the case $\delta_{\mathcal{L}} = 1$, since the state variables $(\mathbf{u}, p)$ is now formally unconstrained `[added corrected function spaces for its rigorous counterpart]`, the derivative of the Lagrangian w.r.t. $(\mathbf{u}, p)$ has to vanish at any optimal point, say e.g. $(\mathbf{u}^\star, p^\star, \Omega^\star)$, i.e.,

$$D_{(\mathbf{u},p)} L_{\mathcal{L}}(\mathbf{u}^\star, p^\star, \Omega^\star, \mathbf{v}, q, \mathbf{v}_{\rm bc})(\tilde{\mathbf{u}}, \tilde{p}) = 0, \ \forall (\tilde{\mathbf{u}}, \tilde{p}).$$

Combine this with

$$D_{(\mathbf{u},p)} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})(\tilde{\mathbf{u}}, \tilde{p}) = D_{\mathbf{u}} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})\tilde{\mathbf{u}} + D_p L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})\tilde{p}, \ \forall (\tilde{\mathbf{u}}, \tilde{p}),$$

then obtain

$$D_{\mathbf{u}} L_{\mathcal{L}}(\mathbf{u}^\star, p^\star, \Omega^\star, \mathbf{v}, q, \mathbf{v}_{\rm bc})\tilde{\mathbf{u}} + D_p L_{\mathcal{L}}(\mathbf{u}^\star, p^\star, \Omega^\star, \mathbf{v}, q, \mathbf{v}_{\rm bc})\tilde{p} = 0, \ \forall (\tilde{\mathbf{u}}, \tilde{p}).$$

Motivated by this stationary equation, choose the adjoint variables/Lagrange multipliers $(\mathbf{v}, q, \mathbf{v}_{\rm bc})$ s.t.

$$\boxed{D_{\mathbf{u}} L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})\tilde{\mathbf{u}} + D_p L_{\mathcal{L}}(\mathbf{u}, p, \Omega, \mathbf{v}, q, \mathbf{v}_{\rm bc})\tilde{p} = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p}).}$$

Expand this more explicitly for all $(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p})$:

$$\begin{aligned}
&\int_\Omega D_{\mathbf{u}} \left(J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \right) \tilde{\mathbf{u}} + D_p \left(J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \right) \tilde{p} {\rm d}\mathbf{x} + \int_\Gamma D_{\mathbf{u}} \left(J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \right) \tilde{\mathbf{u}} + D_p \left(J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \right) \tilde{p}{\rm d}\\
&+ \int_\Omega -D_{\mathbf{u}} \left(\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) - \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \right) \tilde{\mathbf{u}} \cdot \mathbf{v} - D_p \left(\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) - \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \right) \tilde{p} \cdot \mathbf{v}\\
&\qquad + q D_{\mathbf{u}} \left(\nabla\cdot\mathbf{u} + f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \right) \tilde{\mathbf{u}} + q D_p \left(\nabla\cdot\mathbf{u} + f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \right) \tilde{p} {\rm d}\mathbf{x}\\
&- \delta_{\mathcal{L}} \int_\Gamma D_{\mathbf{u}} \left(\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\rm bc}(\mathbf{x}) \right) \tilde{\mathbf{u}} \cdot \mathbf{v}_{\rm bc} + D_p \left(\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{f}_{\rm bc}(\mathbf{x}) \right) \tilde{p} \cdot \mathbf{v}_{\rm bc} {\rm d}\Gamma,
\end{aligned}$$

and more explicitly:

$$\begin{aligned}
&\int_\Omega D_{\mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\tilde{\mathbf{u}} + D_{\nabla\mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\nabla\tilde{\mathbf{u}} + D_p J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\tilde{p}{\rm d}\mathbf{x}\\
&+ \int_\Gamma D_{\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\tilde{\mathbf{u}} + D_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\nabla\tilde{\mathbf{u}} + D_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\tilde{p}{\rm d}\Gamma\\
&+ \int_\Omega -D_{\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\tilde{\mathbf{u}}\cdot\mathbf{v} - D_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v} - D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\Delta\tilde{\mathbf{u}}\cdot\mathbf{v}\\
&\qquad + D_{\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\tilde{\mathbf{u}}\cdot\mathbf{v} + D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}\\
&\qquad - D_p\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\tilde{p}\cdot\mathbf{v} - D_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\nabla\tilde{p}\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\tilde{p}\cdot\mathbf{v}\\
&\qquad + q\nabla\cdot\tilde{\mathbf{u}} + qD_{\mathbf{u}} f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\tilde{\mathbf{u}} + qD_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\nabla\tilde{\mathbf{u}} + qD_p f_{\rm div}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\tilde{p}{\rm d}\mathbf{x}\\
&- \delta_{\mathcal{L}}\int_\Gamma D_{\mathbf{u}}\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc} + D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc} + D_p\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\tilde{p}\cdot\mathbf{v}_{\rm bc}{\rm d}\Gamma = 0, \ \forall(\mathbf{u}
\end{aligned}$$

Question 3.21.2. *Integrate by parts which terms?*

Answer. *All the terms which are the domain integrals containing derivatives of the variations of state variables to transfer their derivatives to the adjoint variables. Roughly speaking:*

$$\int_\Omega \{\nabla\tilde{\mathbf{u}}, \Delta\tilde{\mathbf{u}}, \nabla\tilde{p}\} \cdot \{\mathbf{v}, q\} \,{\rm d}\mathbf{x} \xrightarrow{\text{i.b.p.}} \int_\Omega \{\tilde{\mathbf{u}}, \tilde{p}\} \cdot \{\nabla\mathbf{v}, \Delta\mathbf{v}, \nabla q\} \,{\rm d}\mathbf{x} + \textit{ boundary integrals } \int_\Gamma \cdots {\rm d}\Gamma.$$

The domain integrals on the r.h.s., after gathered appropriately, will yield the adjoint PDEs, meanwhile the boundary integrals, also after gathered appropriately, will yield the adjoint boundary conditions.

$$
\begin{aligned}
&\int_\Omega D_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}} + D_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}} + D_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\mathrm{d}\mathbf{x}\\
&+\int_\Gamma D_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{\mathbf{u}} + D_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}} + D_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{p}\mathrm{d}\Gamma\\
&+\int_\Omega -D_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{\mathbf{u}}\cdot\mathbf{v} - D_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v} - D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\tilde{\mathbf{u}}\cdot\mathbf{v}\\
&\qquad + D_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\cdot\mathbf{v} + D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}\\
&\qquad - D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{p}\cdot\mathbf{v} - D_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\nabla\tilde{p}\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\cdot\mathbf{v}\\
&\qquad + q\nabla\cdot\tilde{\mathbf{u}} + qD_{\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}} + qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}} + qD_p f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{p}\mathrm{d}\mathbf{x}\\
&-\delta_{\mathcal{L}}\int_\Gamma D_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{\mathbf{u}}\cdot\mathbf{v}_{\mathrm{bc}} + D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\mathrm{bc}} + D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\tilde{p}\cdot\mathbf{v}_{\mathrm{bc}}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u}
\end{aligned}
$$

Integrate by parts:

1. Term $D_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}$:

$$
\begin{aligned}
&\int_\Omega D_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = \int_\Omega \nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = \int_\Omega \sum_{i=1}^N\sum_{j=1}^N \partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x}\\
&= \sum_{i=1}^N\sum_{j=1}^N \int_\Omega \partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x} = \sum_{i=1}^N\sum_{j=1}^N -\int_\Omega \partial_{x_i}\partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\mathbf{x} + \int_\Gamma n_i\partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p\\
&= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \sum_{i=1}^N \partial_{x_i}\partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x} + \int_\Gamma \sum_{i=1}^N\sum_{j=1}^N n_i\partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\Gamma\\
&= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \nabla\cdot\left(\nabla_{\nabla u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma\\
&= -\int_\Omega \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma,
\end{aligned}
$$

where $\nabla_{\nabla\mathbf{u}} f(\nabla\mathbf{u}) \coloneqq \left(\partial_{\partial_{x_i}u_j} f(\nabla\mathbf{u})\right)_{i,j=1}^N$ for any scalar function f.

2. Term $-D_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}$:

$$
\begin{aligned}
&-\int_\Omega D_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_\Omega (\nabla_{\nabla\mathbf{u}} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\tilde{\mathbf{u}})_{k=1}^N\cdot\mathbf{v}\mathrm{d}\mathbf{x}\\
&= -\int_\Omega \sum_{k=1}^N \nabla_{\nabla\mathbf{u}} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\tilde{\mathbf{u}}v_k\mathrm{d}\mathbf{x} = -\int_\Omega \sum_{k=1}^N\sum_{i=1}^N\sum_{j=1}^N \partial_{\partial_{x_i}u_j} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{x_i}\tilde{u}_j v_k\mathrm{d}\mathbf{x}\\
&= -\sum_{i=1}^N\sum_{j=1}^N\sum_{k=1}^N \int_\Omega \partial_{\partial_{x_i}u_j} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{x_i}\tilde{u}_j v_k\mathrm{d}\mathbf{x}
\end{aligned}
$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\int_{\Omega}\partial_{x_i}\partial_{\partial_{x_i}u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{u}_j v_k + \partial_{\partial_{x_i}u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{u}_j\partial_{x_i}v_k\mathrm{d}\mathbf{x}$$
$$-\int_{\Gamma}n_i\partial_{\partial_{x_i}u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{u}_j v_k\mathrm{d}\Gamma$$
$$= \int_{\Omega}\sum_{j=1}^{N}\tilde{u}_j\sum_{k=1}^{N}v_k\sum_{i=1}^{N}\partial_{x_i}\partial_{\partial_{x_i}u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \sum_{j=1}^{N}\tilde{u}_j\sum_{k=1}^{N}\sum_{i=1}^{N}\partial_{\partial_{x_i}u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{x_i}v_k\mathrm{d}\mathbf{x}$$
$$-\int_{\Gamma}\sum_{j=1}^{N}\tilde{u}_j\sum_{k=1}^{N}v_k\sum_{i=1}^{N}n_i\partial_{\partial_{x_i}u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathrm{d}\Gamma$$
$$= \int_{\Omega}\sum_{j=1}^{N}\tilde{u}_j\sum_{k=1}^{N}v_k\nabla\cdot\left(\nabla_{\nabla u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\right) + \sum_{j=1}^{N}\tilde{u}_j\sum_{k=1}^{N}\nabla_{\nabla u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\nabla v_k\mathrm{d}\mathbf{x}$$
$$-\int_{\Gamma}\sum_{j=1}^{N}\tilde{u}_j\sum_{k=1}^{N}v_k\nabla_{\nabla u_j}P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n}\mathrm{d}\Gamma$$
$$= \int_{\Omega}\sum_{j=1}^{N}\tilde{u}_j\nabla\cdot\left(\nabla_{\nabla u_j}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\right)\cdot\mathbf{v} + \sum_{j=1}^{N}\tilde{u}_j\nabla_{\nabla u_j}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p):\nabla\mathbf{v}\mathrm{d}\mathbf{x}$$
$$-\int_{\Gamma}\sum_{j=1}^{N}\tilde{u}_j\left(\nabla_{\nabla u_j}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n}\right)\cdot\mathbf{v}\mathrm{d}\Gamma$$
$$= \int_{\Omega}(\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p))\cdot\mathbf{v})\cdot\tilde{\mathbf{u}} + (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p):\nabla\mathbf{v})\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}$$
$$-\int_{\Gamma}((\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n})\cdot\mathbf{v})\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma.$$

3. Term $D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\tilde{\mathbf{u}}\cdot\mathbf{v}$:

$$-\int_{\Omega}D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_{\Omega}\left(\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\right)_{i,j=1}^{N}\Delta\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\mathbf{x}$$
$$= -\int_{\Omega}\left(\sum_{j=1}^{N}\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\tilde{u}_j\right)_{j=1}^{N}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_{\Omega}\sum_{i=1}^{N}\sum_{j=1}^{N}\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\tilde{u}_j v_i\mathrm{d}\mathbf{x}$$
$$= -\sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\Omega}\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\tilde{u}_j v_i\mathrm{d}\mathbf{x}$$
$$= -\sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\Omega}\tilde{u}_j\Delta\left(\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)v_i\right)\mathrm{d}\mathbf{x}$$
$$+\int_{\Gamma}\partial_{\mathbf{n}}\tilde{u}_j\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)v_i - \tilde{u}_j\partial_{\mathbf{n}}\left(\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)v_i\right)\mathrm{d}\Gamma$$
$$= -\sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\Omega}\tilde{u}_j\Delta\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)v_i + \tilde{u}_j\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta v_i\mathrm{d}\mathbf{x}$$
$$+\int_{\Gamma}\partial_{\mathbf{n}}\tilde{u}_j\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)v_i - \tilde{u}_j\partial_{\mathbf{n}}\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)v_i - \tilde{u}_j\partial_{\Delta u_j}P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}$$

$$= -\int_\Omega \sum_{i=1}^N \sum_{j=1}^N v_i \Delta \partial_{\Delta u_j} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{u}_j + \Delta v_i \partial_{\Delta u_j} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{u}_j \mathrm{d}\mathbf{x}$$

$$+ \int_\Gamma \sum_{i=1}^N \sum_{j=1}^N v_i \partial_{\Delta u_j} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\tilde{u}_j - \sum_{i=1}^N \sum_{j=1}^N v_i \partial_{\mathbf{n}} \partial_{\Delta u_j} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{u}_j$$

$$- \sum_{i=1}^N \sum_{j=1}^N \partial_{\mathbf{n}} v_i \partial_{\Delta u_j} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{u}_j \mathrm{d}\Gamma$$

$$= -\int_\Omega \mathbf{v}^\top \Delta D_{\boldsymbol{\Delta}\mathbf{u}} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{\mathbf{u}} + \boldsymbol{\Delta}\mathbf{v}^\top D_{\boldsymbol{\Delta}\mathbf{u}} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{\mathbf{u}} \mathrm{d}\mathbf{x}$$

$$+ \int_\Gamma \mathbf{v}^\top D_{\boldsymbol{\Delta}\mathbf{u}} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\tilde{\mathbf{u}} - \mathbf{v}^\top \partial_{\mathbf{n}} D_{\boldsymbol{\Delta}\mathbf{u}} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\tilde{\mathbf{u}} - \partial_{\mathbf{n}}\mathbf{v}^\top D_{\boldsymbol{\Delta}\mathbf{u}} \mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)$$

4. Term $D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}$:

$$\int_\Omega D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \left(\nabla_{\nabla\mathbf{u}} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\tilde{\mathbf{u}}\right)_{k=1}^N \cdot \mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \sum_{k=1}^N \nabla_{\nabla\mathbf{u}} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\tilde{\mathbf{u}} v_k \mathrm{d}\mathbf{x}$$

$$= \int_\Omega \sum_{k=1}^N \sum_{i=1}^N \sum_{j=1}^N \partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j v_k \mathrm{d}\mathbf{x} = \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N \int_\Omega \partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j v_k \mathrm{d}\mathbf{x}$$

$$= \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N - \int_\Omega \partial_{x_i}\partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j v_k + \partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j \partial_{x_i} v_k \mathrm{d}\mathbf{x} + \int_\Gamma n_i \partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j v_k \mathrm{d}\Gamma$$

$$= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N v_k \sum_{i=1}^N \partial_{x_i}\partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N \sum_{i=1}^N \partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i} v_k \mathrm{d}\mathbf{x}$$

$$+ \int_\Gamma \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N v_k \sum_{i=1}^N n_i \partial_{\partial_{x_i} u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\Gamma$$

$$= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N v_k \nabla\cdot\big(\nabla_{\nabla u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\big) + \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N \nabla_{\nabla u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\nabla v_k \mathrm{d}\mathbf{x}$$

$$+ \int_\Gamma \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N v_k \nabla_{\nabla u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n}\mathrm{d}\Gamma$$

$$= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \nabla\cdot\big(\nabla_{\nabla u_j}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\big)\cdot\mathbf{v} + \sum_{j=1}^N \tilde{u}_j \nabla_{\nabla u_j}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v}\mathrm{d}\mathbf{x} + \int_\Gamma \sum_{j=1}^N \tilde{u}_j \left(\nabla_{\nabla u_j}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n}\right)\cdot$$

$$= -\int_\Omega \left(\nabla\cdot\left(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\cdot\mathbf{v}\right)\cdot\tilde{\mathbf{u}} + \left(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v}\right)\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma \left(\left(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n}\right)\cdot\mathbf{v}\right)\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma.$$

5. Term $-D_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\nabla\tilde{p}\cdot\mathbf{v}$:

$$-\int_\Omega D_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\nabla\tilde{p}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_\Omega \left(\sum_{j=1}^N \partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\partial_{x_j}\tilde{p}\right)_{i=1}^N \cdot\mathbf{v}\mathrm{d}\mathbf{x}$$

$$= -\int_\Omega \sum_{i=1}^N \sum_{j=1}^N v_i \partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\partial_{x_j}\tilde{p}\mathrm{d}\mathbf{x} = -\sum_{i=1}^N \sum_{j=1}^N \int_\Omega v_i \partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\boldsymbol{\Delta}\mathbf{u},p,\nabla p)\partial_{x_j}\tilde{p}\mathrm{d}\mathbf{x}$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\Omega} \partial_{x_j} v_i \partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{p} + v_i \partial_{x_j}\partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\tilde{p}\mathrm{d}\mathbf{x} - \int_{\Gamma} v_i \partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta$$

$$= \int_{\Omega} \tilde{p}\sum_{i=1}^{N}\sum_{j=1}^{N} \partial_{x_i} v_j \partial_{\partial_{x_i} p} P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \tilde{p}\sum_{i=1}^{N} v_i \sum_{j=1}^{N} \partial_{x_j}\partial_{\partial_{x_j} p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathrm{d}\mathbf{x}$$

$$- \int_{\Gamma} \tilde{p}\sum_{i=1}^{N}\sum_{j=1}^{N} n_i \partial_{\partial_{x_j} p} P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) v_j \mathrm{d}\Gamma$$

$$= \int_{\Omega} \tilde{p}\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} + \tilde{p}\sum_{i=1}^{N} v_i \nabla\cdot\left(\nabla_{\nabla p} P_i(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\right)\mathrm{d}\mathbf{x} - \int_{\Gamma} \tilde{p}\mathbf{n}^{\top}\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta$$

$$= \int_{\Omega} \tilde{p}\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} + \tilde{p}\nabla\cdot\left(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\right)\cdot\mathbf{v}\mathrm{d}\mathbf{x} - \int_{\Gamma} \tilde{p}\mathbf{n}^{\top}\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,$$

6. Term $q\nabla\cdot\tilde{\mathbf{u}}$: Use (ibp),

$$\int_{\Omega} q\nabla\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = -\int_{\Omega}\nabla q\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_{\Gamma} q\tilde{\mathbf{u}}\cdot\mathbf{n}\mathrm{d}\Gamma.$$

7. Term $qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}$:

$$\int_{\Omega} qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = \int_{\Omega} q\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}$$

$$= \int_{\Omega} q\sum_{i=1}^{N}\sum_{j=1}^{N}\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x} = \sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\Omega} q\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x}$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N} -\int_{\Omega}\partial_{x_i} q\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j + q\partial_{x_i}\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\mathbf{x} + \int_{\Gamma} qn_i\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\Gamma$$

$$= -\int_{\Omega}\sum_{i=1}^{N}\sum_{j=1}^{N}\partial_{x_i} q\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j + q\sum_{j=1}^{N}\tilde{u}_j\sum_{i=1}^{N}\partial_{x_i}\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x}$$

$$+ \int_{\Gamma} q\sum_{i=1}^{N}\sum_{j=1}^{N} n_i\partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\Gamma$$

$$= -\int_{\Omega}\nabla^{\top} q\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}} + q\sum_{j=1}^{N}\tilde{u}_j\nabla\cdot\left(\nabla_{\nabla u_j}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x} + \int_{\Gamma} q\mathbf{n}^{\top}\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma$$

$$= -\int_{\Omega}\nabla^{\top} q\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}} + q\left(\nabla\cdot\left(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\right)\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_{\Gamma} q\mathbf{n}^{\top}\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma.$$

Gather terms:

$$\begin{aligned}
&\int_\Omega [\nabla_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) - \nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p\\
&\qquad + \nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} - \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v}\\
&\qquad + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v} - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v} - \nabla q + q\nabla_{\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\\
&\qquad -\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\nabla q - q\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}\\
&+\int_\Omega \tilde{p}\,[D_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{v} + \nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v}\\
&\qquad +\nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p))\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_p f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathrm{d}\mathbf{x}\\
&+\int_\Gamma [\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n})\cdot\mathbf{v}\\
&\qquad - \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v} + q\mathbf{n}\\
&\qquad +q\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} - \delta_{\mathcal{L}}\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\rm bc}]\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma\\
&+\int_\Gamma \tilde{p}\left[D_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - \delta_{\mathcal{L}} D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\rm bc}\right]\mathrm{d}\Gamma\\
&+\int_\Gamma \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \nabla\tilde{\mathbf{u}} + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\tilde{\mathbf{u}}\\
&\qquad - \delta_{\mathcal{L}} D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc}\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}).
\end{aligned}\tag{EuLa-gfld}$$

Since this equation holds for all variations $(\tilde{\mathbf{u}},\tilde{p})$, consider the following 2 cases:

- **Case $\delta_{\mathcal{L}} = 0$.** This means to "activate" the boundary-condition constraint $\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\rm bc}(\mathbf{x})$ on Γ, so it will not be penalized by the Lagrangian L. To simplify further the last equation, we define $\Gamma_{\rm v}^{\mathbf{u}}$ and $\Gamma_{\rm v}^{p}$ as the "varying" components w.r.t. $\mathbf{u}$ and p of Γ, respectively, i.e.,

$$\begin{aligned}
\Gamma_{\rm nv}^{\mathbf{u}} &\coloneqq \{\mathbf{x}\in\Gamma; (\mathbf{Q}(\mathbf{x},\mathbf{u}+\tilde{\mathbf{u}},\nabla\mathbf{u}+\nabla\tilde{\mathbf{u}},p+\tilde{p},\mathbf{n},\mathbf{t}) = \mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})) \Rightarrow \tilde{\mathbf{u}} = \mathbf{0}\},\\
\Gamma_{\rm nv}^{p} &\coloneqq \{\mathbf{x}\in\Gamma; (\mathbf{Q}(\mathbf{x},\mathbf{u}+\tilde{\mathbf{u}},\nabla\mathbf{u}+\nabla\tilde{\mathbf{u}},p+\tilde{p},\mathbf{n},\mathbf{t}) = \mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})) \Rightarrow \tilde{p} = 0\},\\
\Gamma_{\rm v}^{\mathbf{u}} &\coloneqq \Gamma\backslash\Gamma_{\rm nv}^{\mathbf{u}},\ \Gamma_{\rm v}^{p} \coloneqq \Gamma\backslash\Gamma_{\rm nv}^{p}.
\end{aligned}$$

E.g., the Dirichlet components of Γ w.r.t. $\mathbf{u}$ and p, denoted by $\Gamma_{\rm D}^{\mathbf{u}}$ and $\Gamma_{\rm D}^{p}$, respectively:

$$\begin{cases}\mathbf{u} = \mathbf{u}_{\rm D}, & \text{on } \Gamma_{\rm D}^{\mathbf{u}},\\ p = p_{\rm D}, & \text{on } \Gamma_{\rm D}^{p}.\end{cases}$$

belong to the "non-variation" components just defined of Γ: $\Gamma_{\rm D}^{\mathbf{u}}\subset\Gamma_{\rm nv}^{\mathbf{u}}$ and $\Gamma_{\rm D}^{p}\subset\Gamma_{\rm nv}^{p}$.

To see the general structure, we rewrite (EuLa-gfld) as follows:

$$\begin{aligned}
&\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},\Delta\mathbf{v},q,\nabla q)\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Omega F_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q)\tilde{p}\mathrm{d}\mathbf{x}\\
&\quad + \int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{n},\mathbf{t})\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma + \int_\Gamma F_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t})\tilde{p}\mathrm{d}\Gamma\\
&\quad + \int_\Gamma F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t},\nabla\tilde{\mathbf{u}})\mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}},\tilde{p}),
\end{aligned}\tag{brief-EuLa-gfld}$$

where

$\mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},\Delta\mathbf{v},q,\nabla q)$

$$
\begin{aligned}
&:= \nabla_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) - \nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla \\
&\quad + \nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} - \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v} \\
&\quad + \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{v} - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v} - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v} - \nabla q + q\nabla_{\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \\
&\quad - \nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\nabla q - q\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\,, \\
&F_\Omega^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q) \\
&:= D_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{v} + \nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} \\
&\quad + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p))\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_p f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p), \\
&\mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{n},\mathbf{t}) \\
&:= \nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n})\cdot\mathbf{v} \\
&\quad - \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v} + q\mathbf{n} \\
&\quad + q\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n}, \\
&F_\Gamma^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t}) := D_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}, \\
&F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t},\nabla\tilde{\mathbf{u}}) := \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \nabla\tilde{\mathbf{u}} + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\tilde{\mathbf{u}},
\end{aligned}
$$

for all $(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{n},\mathbf{t},\tilde{\mathbf{u}},\tilde p)$ s.t.

$$\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) = \mathbf{Q}(\mathbf{x},\mathbf{u}+\tilde{\mathbf{u}},\nabla\mathbf{u}+\nabla\tilde{\mathbf{u}},p+\tilde p,\mathbf{n},\mathbf{t}) = \mathbf{f}_{\rm bc}(\mathbf{x}) \text{ on } \Gamma.$$

We now deduce the adjoint equations of (gfld) from (brief-EuLa-gfld) as follows:

- Choose $\tilde{\mathbf{u}} = \mathbf{0}$ in $\overline{\Omega}$, (brief-EuLa-gfld) then becomes

  $$\int_\Omega F_\Omega^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q)\tilde p\,{\rm d}\mathbf{x} + \int_\Gamma F_\Gamma^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t})\tilde p\,{\rm d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde p).$$

  Then choose $\tilde p$ varying s.t. $\tilde p|_\Gamma = 0$, then the last equality yields

  $$\int_\Omega F_\Omega^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q)\tilde p\,{\rm d}\mathbf{x} = 0,\ \forall(\mathbf{u},p,\Omega,\tilde p) \text{ s.t. } \tilde p|_\Gamma = 0.$$

  Hence, $(\mathbf{v},q)$ satisfies

  $$\boxed{F_\Omega^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q) = 0 \text{ in } \Omega.} \tag{3.21.1}$$

  Plug it back in, obtain

  $$\int_\Gamma F_\Gamma^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t})\tilde p\,{\rm d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde p).$$

  Note that $\tilde p|_{\Gamma_{\rm nv}^p} = 0$, the last equality yields

  $$\int_{\Gamma_{\rm v}^p} F_\Gamma^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t})\tilde p\,{\rm d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde p).$$

  Thus, $(\mathbf{v},q)$ satisfies

  $$\boxed{F_\Gamma^{\tilde p}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{n},\mathbf{t}) = 0 \text{ on } \Gamma_{\rm v}^p.} \tag{3.21.2}$$

- Assume that $(\mathbf{v}, q)$ satisfies (3.21.1) and (3.21.2), (brief-EuLa-gfld) then becomes

$$\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, \Delta\mathbf{v}, q, \nabla q) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma$$
$$+ \int_\Gamma F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{n}, \mathbf{t}, \nabla\tilde{\mathbf{u}}) \mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}),$$

Choose $\tilde{\mathbf{u}}$ varying s.t. $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$ and $\nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}$, the last equality yields

$$\int_\Omega \mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, \Delta\mathbf{v}, q, \nabla q) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } \tilde{\mathbf{u}}|_\Gamma = \mathbf{0} \text{ and } \nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}.$$

Hence, $(\mathbf{v}, q)$ satisfies

$$\boxed{\mathbf{F}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, \Delta\mathbf{v}, q, \nabla q) = \mathbf{0} \text{ in } \Omega.} \tag{3.21.3}$$

Plug it back in, obtain

$$\int_\Gamma \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_\Gamma F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{n}, \mathbf{t}, \nabla\tilde{\mathbf{u}}) \mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}})$$

Note that $\tilde{\mathbf{u}}|_{\Gamma_{\mathrm{nv}}^{\mathbf{u}}} = \mathbf{0}$, the last equality yields

$$\int_{\Gamma_{\mathrm{v}}^{\mathbf{u}}} \mathbf{F}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_\Gamma F_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{n}, \mathbf{t}, \nabla\tilde{\mathbf{u}}) \mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}$$

To simplify the last equality further, we need the explicit formula of $\mathbf{P}$ and $\mathbf{Q}$.

Conclude:

$$\begin{cases} -\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\Delta\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)) : \nabla\mathbf{v} \\ \quad - [\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)]\,\mathbf{v} \\ \quad + [\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p))]\cdot\mathbf{v} - \nabla q - \nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\cdot\nabla q \\ \quad + q\,[-\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)) + \nabla_{\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)] = \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)) - \nabla_{\mathbf{u}}J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \\ \nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) : \nabla\mathbf{v} + [-D_p\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)) + D_p\mathbf{f}(\mathbf{x}, \mathbf{u}, \\ \quad = -D_pJ_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) - qD_pf_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \text{ in } \Omega, \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\mathrm{bc}}(\mathbf{x}) \text{ on } \Gamma, \\ \mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v} = D_pJ_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \text{ on } \Gamma_{\mathrm{v}}^p, \\ \displaystyle\int_{\Gamma_{\mathrm{v}}^{\mathbf{u}}} [\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\cdot\mathbf{n} + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) - (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\cdot\mathbf{n})\cdot\mathbf{v} \\ \quad - \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\cdot\mathbf{n})\cdot\mathbf{v} + q\mathbf{n} \\ \quad + q\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\cdot\mathbf{n}]\cdot\tilde{\mathbf{u}}\mathrm{d}\Gamma \\ \quad + \displaystyle\int_\Gamma \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}). \end{cases} \tag{adj-gfld}$$

Remark 3.21.3. *The last integral equation in* (adj-gfld) *seems "overdetermined". Indeed, choose* $\tilde{\mathbf{u}}$ *varying s.t.* $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$*, then* $(\mathbf{v}, q)$ *satisfies*

$$\int_\Gamma \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla\tilde{\mathbf{u}} + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\tilde{\mathbf{u}}\mathrm{d}\Gamma = 0, \ \forall(\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } \tilde{\mathbf{u}}|_\Gamma = \mathbf{0}.$$

The l.h.s. of this equals

$$\begin{aligned}
&\int_\Gamma \sum_{i=1}^N \sum_{j=1}^N \partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j + \sum_{i=1}^N \sum_{j=1}^N v_i \partial_{\Delta u_j} P_i(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) \partial_{\mathbf{n}} \tilde{u}_j \mathrm{d}\Gamma \\
&= \int_\Gamma \sum_{i=1}^N \sum_{j=1}^N \partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j + \sum_{i=1}^N \sum_{j=1}^N v_i \partial_{\Delta u_j} P_i(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) \sum_{k=1}^N n_k \partial_{x_k} \tilde{u}_j \mathrm{d}\Gamma \\
&= \int_\Gamma \sum_{i=1}^N \sum_{j=1}^N \partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j + \sum_{k=1}^N \sum_{j=1}^N v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) \sum_{i=1}^N n_i \partial_{x_i} \tilde{u}_j \mathrm{d}\Gamma \\
&= \int_\Gamma \sum_{i=1}^N \sum_{j=1}^N \left[\partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \sum_{k=1}^N v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) n_i \right] \partial_{x_i} \tilde{u}_j \mathrm{d}\Gamma,
\end{aligned}$$

hence

$$\int_\Gamma \sum_{i=1}^N \sum_{j=1}^N \left[\partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \sum_{k=1}^N v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) n_i \right] \partial_{x_i} \tilde{u}_j \mathrm{d}\Gamma = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \ s.t. \ \tilde{\mathbf{u}}|_\Gamma =$$

This implies that

$$\partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \sum_{k=1}^N v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) n_i = 0, \ \forall i, j = 1, \ldots, N.$$

To determine $\mathbf{v}$*, we only need to solve one of the following* N *linear equations:*

$$\forall j = 1, \ldots, N, \ j^{\text{th}} \ \textit{linear system}: \ \sum_{k=1}^N v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) n_i = -\partial_{\partial_{x_i} u_j} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}), \ \forall i = 1, \ldots,$$

- **Case $\delta_{\mathcal{L}} = 1$.** This means to "deactivate" the boundary-condition constraint $\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) = \mathbf{f}_{\text{bc}}(\mathbf{x})$ on Γ, so it will be penalized by the extended Lagrangian $\mathcal{L}$.

  Again, to see the general structure, we rewrite (EuLa-gfld) as follows:

$$\begin{aligned}
&\int_\Omega \boldsymbol{\mathcal{F}}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, \Delta\mathbf{v}, q, \nabla q) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x} + \int_\Omega \mathcal{F}_\Omega^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q) \tilde{p} \mathrm{d}\mathbf{x} \\
&\quad + \int_\Gamma \boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, q, \mathbf{v}_{\text{bc}}, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_\Gamma \mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{v}_{\text{bc}}, \mathbf{n}, \mathbf{t}) \tilde{p} \mathrm{d}\Gamma \\
&\quad + \int_\Gamma \mathcal{F}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{v}_{\text{bc}}, \mathbf{n}, \mathbf{t}, \nabla\tilde{\mathbf{u}}) \mathrm{d}\Gamma = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}, \tilde{p}),
\end{aligned} \tag{brief-exEuLa-gfld}$$

  where

$$\begin{aligned}
&\boldsymbol{\mathcal{F}}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p, \mathbf{v}, \nabla\mathbf{v}, \Delta\mathbf{v}, q, \nabla q) \\
&\quad := \nabla_{\mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) - \nabla \cdot (\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)) - \nabla_{\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v} + \nabla \cdot (\nabla_{\nabla\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla \\
&\qquad + \nabla_{\nabla\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p) : \nabla\mathbf{v} - \Delta\nabla_{\Delta\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\Delta\mathbf{v} \\
&\qquad + \nabla_{\mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\mathbf{v} - \nabla \cdot (\nabla_{\nabla\mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)) \cdot \mathbf{v} - \nabla_{\nabla\mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) : \nabla\mathbf{v} - \nabla q + q\nabla_{\mathbf{u}} f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \\
&\qquad - \nabla_{\nabla\mathbf{u}} f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) \cdot \nabla q - q\nabla \cdot (\nabla_{\nabla\mathbf{u}} f_{\text{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)),
\end{aligned}$$

$$
\begin{aligned}
&\mathcal{F}_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q)\\
&\quad := D_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{v} + \nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v}\\
&\qquad + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p))\cdot\mathbf{v} + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v} + qD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p),\\
&\boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t})\\
&\quad := \nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n})\cdot\mathbf{v}\\
&\qquad - \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v} + q\mathbf{n}\\
&\qquad + q\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} - \nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\rm bc},\\
&\mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t}) := D_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - \mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} - D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p\\
&\mathcal{F}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t},\nabla\tilde{\mathbf{u}})\\
&\quad := \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \nabla\tilde{\mathbf{u}} + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\tilde{\mathbf{u}} - D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}_{\rm bc},
\end{aligned}
$$

for all $(\mathbf{x},\mathbf{u},p,\mathbf{v},q,\mathbf{n},\mathbf{t},\tilde{\mathbf{u}},\tilde{p})$.

We now deduce the adjoint equations of (gfld) from (brief-exEuLa-gfld) as follows:

- Choose $\tilde{\mathbf{u}} = \mathbf{0}$ in $\overline{\Omega}$, (brief-exEuLa-gfld) then becomes

$$\int_\Omega \mathcal{F}_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q)\tilde{p}{\rm d}\mathbf{x} + \int_\Gamma \mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t})\tilde{p}{\rm d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{p}).$$

  Then choose $\tilde{p}$ varying s.t. $\tilde{p}|_\Gamma = 0$, then the last equality yields

$$\int_\Omega \mathcal{F}_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q)\tilde{p}{\rm d}\mathbf{x} = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{p}) \text{ s.t. } \tilde{p}|_\Gamma = 0.$$

  Hence, $(\mathbf{v},q)$ satisfies

$$\boxed{\mathcal{F}_\Omega^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q) = 0 \text{ in } \Omega.} \tag{3.21.4}$$

  Plug it back in, obtain

$$\int_\Gamma \mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t})\tilde{p}{\rm d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{p}).$$

  Unlike the previous case, $\tilde{p}$ can vary on the whole of Γ, hence the last equality implies that $(\mathbf{v},q)$ satisfies

$$\boxed{\mathcal{F}_\Gamma^{\tilde{p}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t}) = 0 \text{ on } \Gamma.} \tag{3.21.5}$$

- Assume that $(\mathbf{v},q)$ satisfies (3.21.4) and (3.21.5), (brief-exEuLa-gfld) then becomes

$$
\begin{aligned}
&\int_\Omega \boldsymbol{\mathcal{F}}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},\Delta\mathbf{v},q,\nabla q)\cdot\tilde{\mathbf{u}}{\rm d}\mathbf{x} + \int_\Gamma \boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t})\cdot\tilde{\mathbf{u}}{\rm d}\Gamma\\
&\quad + \int_\Gamma \mathcal{F}_\Gamma^{\nabla\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\mathbf{v}_{\rm bc},\mathbf{n},\mathbf{t},\nabla\tilde{\mathbf{u}}){\rm d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}).
\end{aligned}
$$

  Choose $\tilde{\mathbf{u}}$ varying s.t. $\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}$ and $\nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}$, the last equality yields

$$\int_\Omega \boldsymbol{\mathcal{F}}_\Omega^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},\Delta\mathbf{v},q,\nabla q)\cdot\tilde{\mathbf{u}}{\rm d}\mathbf{x} = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}) \text{ s.t. } \tilde{\mathbf{u}}|_\Gamma = \mathbf{0} \text{ and } \nabla\tilde{\mathbf{u}}|_\Gamma = \mathbf{0}_{N\times N}.$$

Hence, $(\mathbf{v}, q)$ satisfies

$$\boxed{\boldsymbol{\mathcal{F}}_{\Omega}^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p, \mathbf{v}, \nabla \mathbf{v}, \Delta \mathbf{v}, q, \nabla q) = \mathbf{0} \text{ in } \Omega.}$$

Plug it back in, obtain

$$\int_{\Gamma} \boldsymbol{\mathcal{F}}_{\Gamma}^{\tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p, \mathbf{v}, \nabla \mathbf{v}, q, \mathbf{v}_{\rm bc}, \mathbf{n}, \mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma + \int_{\Gamma} \mathcal{F}_{\Gamma}^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{v}_{\rm bc}, \mathbf{n}, \mathbf{t}, \nabla \tilde{\mathbf{u}}) \mathrm{d}\Gamma = 0, \ \forall (\mathbf{u}$$

Choose $\tilde{\mathbf{u}}$ varying s.t. $\tilde{\mathbf{u}}|_{\Gamma} = \mathbf{0}$, the last equality then becomes

$$\int_{\Gamma} \mathcal{F}_{\Gamma}^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{v}_{\rm bc}, \mathbf{n}, \mathbf{t}, \nabla \tilde{\mathbf{u}}) \mathrm{d}\Gamma = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{\mathbf{u}}) \text{ s.t. } \tilde{\mathbf{u}}|_{\Gamma} = \mathbf{0}.$$

The l.h.s. equals

$$\begin{aligned}
&\int_{\Gamma} \mathcal{F}_{\Gamma}^{\nabla \tilde{\mathbf{u}}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p, \mathbf{v}, \mathbf{v}_{\rm bc}, \mathbf{n}, \mathbf{t}, \nabla \tilde{\mathbf{u}}) \mathrm{d}\Gamma \\
&= \int_{\Gamma} \nabla_{\nabla \mathbf{u}} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla \tilde{\mathbf{u}} + \mathbf{v}^{\top} D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \partial_{\mathbf{n}} \tilde{\mathbf{u}} - D_{\nabla \mathbf{u}} \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \nabla \tilde{\mathbf{u}} \cdot \mathbf{v}_{\rm bc} \mathrm{d}\Gamma \\
&= \int_{\Gamma} \sum_{i=1}^{N} \sum_{j=1}^{N} \partial_{\partial_{x_i} u_j} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j + \sum_{i=1}^{N} \sum_{j=1}^{N} v_i \partial_{\Delta u_j} P_i(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \partial_{\mathbf{n}} \tilde{u}_j \\
&\qquad - \sum_{k=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j v_{{\rm bc},k} \mathrm{d}\Gamma \\
&= \int_{\Gamma} \sum_{i=1}^{N} \sum_{j=1}^{N} \partial_{\partial_{x_i} u_j} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j + \sum_{i=1}^{N} \sum_{j=1}^{N} v_i \partial_{\Delta u_j} P_i(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \sum_{k=1}^{N} n_k \partial_{x_k} \tilde{u}_j \\
&\qquad - \sum_{i=1}^{N} \sum_{j=1}^{N} \partial_{x_i} \tilde{u}_j \sum_{k=1}^{N} \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) v_{{\rm bc},k} \mathrm{d}\Gamma \\
&= \int_{\Gamma} \sum_{i=1}^{N} \sum_{j=1}^{N} \partial_{\partial_{x_i} u_j} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \partial_{x_i} \tilde{u}_j + \sum_{k=1}^{N} \sum_{j=1}^{N} v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \sum_{i=1}^{N} n_i \partial_{x_i} \tilde{u}_j \\
&\qquad - \sum_{i=1}^{N} \sum_{j=1}^{N} \partial_{x_i} \tilde{u}_j \sum_{k=1}^{N} \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) v_{{\rm bc},k} \mathrm{d}\Gamma \\
&= \int_{\Gamma} \sum_{i=1}^{N} \sum_{j=1}^{N} \Bigg[\partial_{\partial_{x_i} u_j} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \sum_{k=1}^{N} v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) n_i \\
&\qquad\qquad - \sum_{k=1}^{N} \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) v_{{\rm bc},k} \Bigg] \partial_{x_i} \tilde{u}_j \mathrm{d}\Gamma,
\end{aligned}$$

hence

$$\begin{aligned}
&\int_{\Gamma} \sum_{i=1}^{N} \sum_{j=1}^{N} \Bigg[\partial_{\partial_{x_i} u_j} J_{\Gamma}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \sum_{k=1}^{N} v_k \partial_{\Delta u_j} P_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) n_i \\
&\qquad\qquad - \sum_{k=1}^{N} \partial_{\partial_{x_i} u_j} Q_k(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) v_{{\rm bc},k} \Bigg] \partial_{x_i} \tilde{u}_j \mathrm{d}\Gamma = 0, \ \forall (\mathbf{u}, p, \Omega, \tilde{u}) \text{ s.t. } \tilde{\mathbf{u}}|_{\Gamma} = \mathbf{0}.
\end{aligned}$$

This implies that

$$\partial_{\partial_{x_i}u_j} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \sum_{k=1}^{N} v_k \partial_{\Delta u_j} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) n_i - \sum_{k=1}^{N} \partial_{\partial_{x_i}u_j} Q_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) v_{\mathrm{bc},k} = 0,\ \forall i,$$

or equivalently,

$$\boxed{\sum_{k=1}^{N} v_k \partial_{\Delta u_j} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) n_i - \partial_{\partial_{x_i}u_j} Q_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) v_{\mathrm{bc},k} = -\partial_{\partial_{x_i}u_j} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}),\ \forall i,j =}$$

Assume that the last equality holds, then plug it back in to obtain:

$$\int_\Gamma \boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) \cdot \tilde{\mathbf{u}} \mathrm{d}\Gamma = 0,\ \forall(\mathbf{u},p,\Omega,\tilde{\mathbf{u}}),$$

hence $(\mathbf{v},q,\mathbf{v}_{\mathrm{bc}})$ satisfies

$$\boxed{\boldsymbol{\mathcal{F}}_\Gamma^{\tilde{\mathbf{u}}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p,\mathbf{v},\nabla\mathbf{v},q,\mathbf{v}_{\mathrm{bc}},\mathbf{n},\mathbf{t}) = \mathbf{0} \text{ on } \Gamma.}$$

Conclude:

$$\begin{cases} -\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v} + (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) : \nabla\mathbf{v} \\ \qquad - \left[\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right]\mathbf{v} \\ \qquad + \left[\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\right]\cdot\mathbf{v} - \nabla q - \nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\nabla q \\ \qquad + q\left[-\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) + \nabla_{\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right] = \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) - \nabla_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \\ \nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} + \left[-D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) + D_p\mathbf{f}(\mathbf{x},\mathbf{u}, \right. \\ \qquad = -D_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - q D_p f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \text{ in } \Omega, \\ -\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} + \left[(-\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{n}\right]\cdot\mathbf{v} \\ \qquad - \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + q\mathbf{n} - \nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\mathrm{bc}} \\ \qquad = -\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} - \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) - q\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} \text{ on } \Gamma, \\ \mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{v}_{\mathrm{bc}} = D_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) \text{ on } \Gamma, \\ \sum_{k=1}^{N} v_k\partial_{\Delta u_j} P_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) n_i - \partial_{\partial_{x_i}u_j} Q_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) v_{\mathrm{bc},k} = -\partial_{\partial_{x_i}u_j} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}),\ \forall i,j = 1,\ldots \end{cases} \tag{ex-adj-gfld}$$

Remark 3.21.4. *The last equation in (ex-adj-gfld) can be simplified further when the explicit form of* $\mathbf{P}$ *and* $\mathbf{Q}$ *are given.*

3.21.6 Weak formulation of adjoint equations of (gfld)*

Test the 1st 2 equations of (adj-gfld) with $\mathbf{w}$ and r, respectively, over Ω:

$$\begin{cases} \displaystyle\int_\Omega \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v}\cdot\mathbf{w} + (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) : \nabla\mathbf{v}\cdot\mathbf{w} \\ \qquad - [\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathbf{v}\cdot\mathbf{w} \\ \qquad + [[\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{v}]\cdot\mathbf{w} - \nabla q\cdot\mathbf{w} + (\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\,\cdot \\ \qquad + q\,[\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) - \nabla_{\mathbf{u}}f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{w}{\rm d}\mathbf{x} \\ \quad = \displaystyle\int_\Omega \nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{w} - \nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{w}{\rm d}\mathbf{x}, \\ \displaystyle\int_\Omega r\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} \\ \qquad + r\,[-D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{v}{\rm d}\mathbf{x} \\ \quad = \displaystyle\int_\Omega -rD_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + qrD_pf_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p){\rm d}\mathbf{x}. \end{cases}$$

Integrate by parts:

1. Term $\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v}\cdot\mathbf{w}$:

$$\int_\Omega -\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v}\cdot\mathbf{w}{\rm d}\mathbf{x} = \int_\Omega \left(\sum_{j=1}^N \partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta v_j\right)_{i=1}^N\cdot\mathbf{w}{\rm d}\mathbf{x}$$

$$= \int_\Omega\sum_{i=1}^N\sum_{j=1}^N w_i\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta v_j{\rm d}\mathbf{x} = \sum_{i=1}^N\sum_{j=1}^N\int_\Omega w_i\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta v_j{\rm d}\mathbf{x}$$

$$= \sum_{i=1}^N\sum_{j=1}^N - \int_\Omega \nabla v_j\cdot\nabla w_i\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla v_j\cdot\nabla\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)w_i{\rm d}\mathbf{x}$$
$$+ \int_\Gamma \partial_{\mathbf{n}}v_jw_i\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p){\rm d}\Gamma$$

$$= -\int_\Omega\sum_{j=1}^N\nabla v_j\cdot\sum_{i=1}^N\nabla w_i\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \sum_{j=1}^N\nabla v_j\cdot\sum_{i=1}^N w_i\nabla\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p){\rm d}\mathbf{x}$$
$$+ \int_\Gamma\sum_{i=1}^N\sum_{j=1}^N w_i\partial_{\Delta u_i}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}v_j{\rm d}\Gamma$$

$$= -\int_\Omega\sum_{j=1}^N\nabla v_j\cdot(\nabla_{\Delta\mathbf{u}}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\nabla\mathbf{w}) + \sum_{j=1}^N\nabla v_j\cdot(\nabla\nabla_{\Delta\mathbf{u}}P_j(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{w})\,{\rm d}\mathbf{x}$$
$$+ \int_\Gamma \mathbf{w}^\top\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v}{\rm d}\Gamma$$
$$= -\int_\Omega \nabla\mathbf{v} : (\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\nabla\mathbf{w}) + \nabla\mathbf{v} : (\nabla\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{w})\,{\rm d}\mathbf{x}$$
$$+ \int_\Gamma \mathbf{w}^\top\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v}{\rm d}\Gamma.$$

2. Term $-\nabla q \cdot \mathbf{w}$:

$$-\int_\Omega \nabla q \cdot \mathbf{w} \mathrm{d}\mathbf{x} = \int_\Omega q \nabla \cdot \mathbf{w} \mathrm{d}\mathbf{x} - \int_\Gamma q \mathbf{w} \cdot \mathbf{n} \mathrm{d}\Gamma.$$

3. Term $(\nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \nabla q) \cdot \mathbf{w}$:

$$\begin{aligned}
&\int_\Omega (\nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \nabla q) \cdot \mathbf{w} \mathrm{d}\mathbf{x} = \int_\Omega \nabla^\top q \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{w} \mathrm{d}\mathbf{x} \\
&= \int_\Omega \sum_{i=1}^N \sum_{j=1}^N \partial_{x_i} q \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) w_j \mathrm{d}\mathbf{x} = \sum_{i=1}^N \sum_{j=1}^N \int_\Omega \partial_{x_i} q \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) w_j \mathrm{d}\mathbf{x} \\
&= \sum_{i=1}^N \sum_{j=1}^N - \int_\Omega q \partial_{x_i} \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) w_j + q \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \partial_{x_i} w_j \mathrm{d}\mathbf{x} + \int_\Gamma q n_i \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) w_j \mathrm{d}\Gamma \\
&= - \int_\Omega q \sum_{j=1}^N w_j \sum_{i=1}^N \partial_{x_i} \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) + q \sum_{i=1}^N \sum_{j=1}^N \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \partial_{x_i} w_j \mathrm{d}\mathbf{x} \\
&\quad + \int_\Gamma q \sum_{i=1}^N \sum_{j=1}^N n_i \partial_{\partial_{x_i} u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) w_j \mathrm{d}\Gamma \\
&= - \int_\Omega q \sum_{j=1}^N w_j \nabla \cdot \big(\nabla_{\nabla u_j} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \big) + q \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) : \nabla \mathbf{w} \mathrm{d}\mathbf{x} + \int_\Gamma q \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{w} \mathrm{d}\Gamma \\
&= - \int_\Omega q \nabla \cdot (\nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \cdot \mathbf{w} + q \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) : \nabla \mathbf{w} \mathrm{d}\mathbf{x} + \int_\Gamma q \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{w} \mathrm{d}\Gamma.
\end{aligned}$$

Plug in to obtain:

$$\begin{aligned}
&\int_\Omega -\nabla \mathbf{v} : (\nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \cdot \nabla \mathbf{w}) + \nabla \mathbf{v} : (\nabla \nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \cdot \mathbf{w}) \\
&\qquad + (\nabla_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) + \nabla_{\nabla \mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) : \nabla \mathbf{v} \cdot \mathbf{w} \\
&\qquad - [\nabla_{\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) + \Delta \nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) - \nabla_{\mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)] \, \mathbf{v} \cdot \mathbf{w} \\
&\qquad + [[\nabla \cdot (\nabla_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p)) - \nabla \cdot (\nabla_{\nabla \mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p))] \cdot \mathbf{v}] \cdot \mathbf{w} + q \nabla \cdot \mathbf{w} - q \nabla \cdot (\nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p \\
&\qquad + q \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) : \nabla \mathbf{w} + q \, [\nabla \cdot (\nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) - \nabla_{\mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)] \cdot \mathbf{w} \mathrm{d}\mathbf{x} \\
&+ \int_\Gamma \mathbf{w}^\top \nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \partial_{\mathbf{n}} \mathbf{v} - q \mathbf{w} \cdot \mathbf{n} + q \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{w} \mathrm{d}\Gamma \\
&\qquad = \int_\Omega \nabla \cdot (\nabla_{\nabla \mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \cdot \mathbf{w} - \nabla_{\mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \mathbf{w} \mathrm{d}\mathbf{x}.
\end{aligned}$$

Note that

$$\begin{aligned}
&\int_{\Gamma \backslash \Gamma_{\mathrm{D}}^{\mathbf{u}}} \mathbf{w}^\top \nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \partial_{\mathbf{n}} \mathbf{v} - q \mathbf{w} \cdot \mathbf{n} + q \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{w} \mathrm{d}\Gamma \\
&= \int_{\Gamma \backslash \Gamma_{\mathrm{D}}^{\mathbf{u}}} [\nabla_{\nabla \mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \mathbf{n} + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) - (\nabla_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \cdot \mathbf{n}) \cdot \mathbf{v} \\
&\qquad - \partial_{\mathbf{n}} \nabla_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{v} + (\nabla_{\nabla \mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \cdot \mathbf{n}) \cdot \mathbf{v} - \delta_{\mathcal{L}} \nabla_{\mathbf{u}} \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \mathbf{v}_{\mathrm{bc}}] \cdot \mathbf{w} \mathrm{d}\Gamma \\
&\quad + \int_{\Gamma \backslash \Gamma_{\mathrm{D}}^p} r \left[D_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) - \mathbf{n}^\top \nabla_{\nabla p} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{v} - \delta_{\mathcal{L}} D_p \mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{v}_{\mathrm{bc}} \right] \mathrm{d}\Gamma
\end{aligned}$$

$$+\int_\Gamma \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \nabla\mathbf{w} + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{w} - \delta_{\mathcal{L}} D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\mathbf{w}\cdot\mathbf{v}_{\rm bc}\mathrm{d}\Gamma$$

Thus, obtain the following weak formulation of (adj-gfld):

$$\begin{cases} \displaystyle\int_\Omega -\nabla\mathbf{v} : (\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\nabla\mathbf{w}) + \nabla\mathbf{v} : (\nabla\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{w}) \\ \qquad + (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) : \nabla\mathbf{v}\cdot\mathbf{w} \\ \qquad - [\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathbf{v}\cdot\mathbf{w} \\ \qquad + [[\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{v}]\cdot\mathbf{w} + q\nabla\cdot\mathbf{w} - q\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u} \\ \qquad + q\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{w} + q\,[\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) - \nabla_{\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{w}\mathrm{d}\mathbf{x} \\ \quad + \displaystyle\int_\Gamma \mathbf{w}^\top\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} - q\mathbf{w}\cdot\mathbf{n} + q\mathbf{n}^\top\nabla_{\nabla\mathbf{u}} f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{w}\mathrm{d}\Gamma \\ \qquad = \displaystyle\int_\Omega \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{w} - \nabla_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{w}\mathrm{d}\mathbf{x}, \\ \displaystyle\int_\Omega r\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} \\ \qquad + r\,[-D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{v}\mathrm{d}\mathbf{x} \\ \qquad = \displaystyle\int_\Omega qrD_p f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - rD_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x}. \end{cases} \tag{wf-adj-gfld}$$

3.21.7 Shape derivatives of (gfld)-constrained (cost-gfld)

To calculate the shape derivatives of (cost-gfld) under the constraint state equation (gfld), consider the *perturbed cost functional*:

$$J(\mathbf{u}_t,p_t,\Omega_t) := \int_{\Omega_t} J_\Omega(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t)\mathrm{d}\mathbf{x} + \int_{\Gamma_t} J_\Gamma(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t,\mathbf{n}_t,\mathbf{t}_t)\mathrm{d}\Gamma_t, \tag{ptb-cost-gfld}$$

where $(\mathbf{u}_t,p_t)$ denotes the strong/classical solution (if exist and unique) of (gfld) on the perturbed domain $\Omega_t := T_t(V)(\Omega)$, i.e.:

$$\begin{cases} \mathbf{P}(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,\Delta\mathbf{u}_t,p_t,\nabla p_t) = \mathbf{f}(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t) & \text{in } \Omega_t, \\ -\nabla\cdot\mathbf{u}_t = f_{\rm div}(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t) & \text{in } \Omega_t, \\ \mathbf{Q}(\mathbf{x},\mathbf{u}_t,\nabla\mathbf{u}_t,p_t,\mathbf{n}_t,\mathbf{t}_t) = \mathbf{f}_{\rm bc}(\mathbf{x}) & \text{on } \Gamma_t, \end{cases} \tag{ptb-gfld}$$

where $\Gamma_t := \partial\Omega_t$.

Define:

- Local shape derivative:

$$\mathbf{u}'(\mathbf{x};V) := \lim_{t\downarrow 0}\frac{\mathbf{u}_t(\mathbf{x}) - \mathbf{u}(\mathbf{x})}{t},\ p'(\mathbf{x};V) := \lim_{t\downarrow 0}\frac{p_t(\mathbf{x}) - p(\mathbf{x})}{t},\ \forall\mathbf{x}\in D.$$

- Material derivative:

$$\mathrm{d}\mathbf{u}(\mathbf{x};V) := \lim_{t\downarrow 0}\frac{\mathbf{u}_t(\mathbf{x}_t) - \mathbf{u}(\mathbf{x})}{t},\ \mathrm{d}p(\mathbf{x};V) := \lim_{t\downarrow 0}\frac{p_t(\mathbf{x}_t) - p(\mathbf{x})}{t},\ \text{where } \mathbf{x}_t := T_t(V)(\mathbf{x}),\ \forall\mathbf{x}\in D.$$

Now subtracting (ptb-gfld) to (gfld) side by side, taking $\lim_{t\downarrow 0}$, we obtain:

$$\begin{cases} D_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\nabla\mathbf{u}'(\mathbf{x};V) + D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{u}'(\mathbf{x}; \\ \quad + D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)p'(\mathbf{x};V) + D_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\nabla p'(\mathbf{x};V) \\ \qquad = D_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V) + D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V) \text{ in } \Omega, \\ -\nabla\cdot\mathbf{u}'(\mathbf{x};V) = D_{\mathbf{u}}f_{\text{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}f_{\text{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V) + D_pf_{\text{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V) \text{ in } \\ D_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\mathbf{u}'(\mathbf{x};V) + D_p\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V) \\ \quad + D_{\mathbf{n}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{n}'(\mathbf{x};V) + D_{\mathbf{t}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{t}'(\mathbf{x};V) = \mathbf{0} \text{ on } \Gamma. \end{cases} \tag{3.21.6}$$

Now start to compute the 1st-order shape derivative for (cost-gfld). Applying the domain and boundary formulas for the domain and boundary integrals, respectively, yields the following "4 combinations" (2 combinations for each of domain and boundary integrals, but only 2 of 4 presented here for brevity):

$$\begin{aligned} dJ(\mathbf{u},p,\Omega;V) &= \int_\Omega J'_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p;V) + \nabla\cdot(J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0))\,\mathrm{d}\mathbf{x} \\ &\quad + \int_\Gamma J'_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t};V) + \nabla\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right)\cdot V(0) + J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\left(\nabla\cdot V(0) - DV\right. \\ &= \int_\Omega J'_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p;V)\mathrm{d}\mathbf{x} + \int_\Gamma J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0)\cdot\mathbf{n}\mathrm{d}\Gamma \\ &\quad + \int_\Gamma J'_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t};V) + \left[\partial_{\mathbf{n}}(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})) + HJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right]V(0)\cdot\mathbf{n}\mathrm{d}\Gamma. \end{aligned}$$

We now compute these explicitly.

1. *1st representation of shape derivative.*

$$\begin{aligned} & dJ(\mathbf{u},p,\Omega;V) \\ &= \int_\Omega J'_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p;V) + \nabla\cdot(J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0))\,\mathrm{d}\mathbf{x} \\ &\quad + \int_\Gamma J'_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t};V) + \nabla\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right)\cdot V(0) + J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\left(\nabla\cdot V(0) - DV(0)\mathbf{n}\cdot\mathbf{n}\right)\mathrm{d}\Gamma \\ &= \int_\Omega D_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V) + \partial_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V) + \nabla\cdot(J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p \\ &\quad + \int_\Gamma D_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\mathbf{u}'(\mathbf{x};V) + \partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V) \\ &\qquad + D_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{n}'(\mathbf{x};V) + D_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{t}'(\mathbf{x};V) \\ &\qquad + [DJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + D_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\mathbf{u} + D_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\nabla\mathbf{u} + \partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p, \\ &\qquad\quad + D_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\mathbf{n} + D_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\mathbf{t}]\,V(0) \\ &\qquad + J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\left(\nabla\cdot V(0) - DV(0)\mathbf{n}\cdot\mathbf{n}\right)\mathrm{d}\Gamma \\ &= \int_\Omega \nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{u}'(\mathbf{x};V) + \nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\mathbf{u}'(\mathbf{x};V) + \partial_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V) + \nabla\cdot(J_\Omega(\mathbf{x},\mathbf{u},\nabla \\ &\quad + \int_\Gamma \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{u}'(\mathbf{x};V) + \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\nabla\mathbf{u}'(\mathbf{x};V) + \partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V) \\ &\qquad + \nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{n}'(\mathbf{x};V) + \nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\mathbf{t}'(\mathbf{x};V) \\ &\qquad + [\nabla J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\nabla\mathbf{u} + \nabla\nabla\mathbf{u}:\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u}, \end{aligned}$$

$$
\begin{aligned}
&+\nabla\mathbf{n}\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla\mathbf{t} : \nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})] \cdot V(0) \\
&+ J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\,(\nabla\cdot V(0) - DV(0)\mathbf{n}\cdot\mathbf{n})\,\mathrm{d}\Gamma,
\end{aligned}
$$

where we have expanded $\nabla\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right)$ as follows:

$$
\begin{aligned}
&J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) \\
=\,&J(x_1,\dots,x_N,u_1,\dots,u_N,\partial_{x_1}u_1,\dots,\partial_{x_N}u_1,\dots,\partial_{x_1}u_N,\dots,\partial_{x_N}u_N,p,n_1,\dots,n_N,t_{1,1},\dots,t_{1,N},\dots,t_{N-1,1},\dots,t_{N-} \\
&\partial_{x_k}\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right) \\
=\,&\partial_{x_k}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \sum_{i=1}^{N}\partial_{u_i}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\partial_{x_k}u_i \\
&+\sum_{i=1}^{N}\sum_{j=1}^{N}\partial_{\partial_{x_i}u_j}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\partial_{x_k}\partial_{x_i}u_j + \partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\partial_{x_k}p + \sum_{i=1}^{N}\partial_{n_i}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\partial_{x_k}n_i \\
&+\sum_{i=1}^{N-1}\sum_{j=1}^{N}\partial_{t_{i,j}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\partial_{x_k}t_{i,j} \\
=\,&\partial_{x_k}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\partial_{x_k}\mathbf{u} + \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \partial_{x_k}\nabla\mathbf{u} + \partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n}, \\
&+\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\partial_{x_k}\mathbf{n} + \sum_{i=1}^{N-1}\nabla_{\mathbf{t}_i}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\partial_{x_k}\mathbf{t}_i \\
=\,&\partial_{x_k}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\partial_{x_k}\mathbf{u} + \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \partial_{x_k}\nabla\mathbf{u} + \partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n}, \\
&+\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\partial_{x_k}\mathbf{n} + \nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) : \partial_{x_k}\mathbf{t},
\end{aligned}
$$

hence

$$
\begin{aligned}
\nabla\left(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\right) = &\nabla J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla\mathbf{u}\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla\nabla\mathbf{u} : \nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) \\
&+\partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla p + \nabla\mathbf{n}\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla\mathbf{t} : \nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}).
\end{aligned}
$$

Integrate by parts the term $\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{u}'(\mathbf{x};V)$ in $dJ(\mathbf{u},p,\Omega;V)$:

$$
\begin{aligned}
&\int_\Omega \nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x} = \int_\Omega\sum_{i=1}^{N}\sum_{j=1}^{N}\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}u_j'(\mathbf{x};V)\mathrm{d}\mathbf{x} \\
&=\sum_{i=1}^{N}\sum_{j=1}^{N}\int_\Omega\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}u_j'(\mathbf{x};V)\mathrm{d}\mathbf{x} \\
&=\sum_{i=1}^{N}\sum_{j=1}^{N}-\int_\Omega\partial_{x_i}\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)u_j'(\mathbf{x};V)\mathrm{d}\mathbf{x} + \int_\Gamma n_i\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)u_j'(\mathbf{x};V)\mathrm{d}\Gamma \\
&=-\int_\Omega\sum_{i=1}^{N}\sum_{j=1}^{N}\partial_{x_i}\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)u_j'(\mathbf{x};V)\mathrm{d}\mathbf{x} + \int_\Gamma\sum_{i=1}^{N}\sum_{j=1}^{N}n_i\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)u_j'(\mathbf{x};V)\mathrm{d}\Gamma \\
&=-\int_\Omega\sum_{j=1}^{N}u_j'(\mathbf{x};V)\sum_{i=1}^{N}\partial_{x_i}\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x} + \int_\Gamma\mathbf{n}^\top\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma \\
&=-\int_\Omega\sum_{j=1}^{N}u_j'(\mathbf{x};V)\nabla\cdot\left(\nabla_{\nabla u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x} + \int_\Gamma\mathbf{n}^\top\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma
\end{aligned}
$$

$$= -\int_\Omega \nabla \cdot (\nabla_{\nabla \mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)) \cdot \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\Gamma.$$

Then

$$\begin{aligned}
& dJ(\mathbf{u}, p, \Omega; V) \\
= & \int_\Omega [\nabla_{\mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) - \nabla \cdot (\nabla_{\nabla \mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p))] \cdot \mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) p'(\mathbf{x}; V) + \nabla \cdot (J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) V \\
& + \int_\Gamma \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} J_\Omega(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{u}'(\mathbf{x}; V) + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{u}'(\mathbf{x}; V) + \nabla_{\nabla \mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla \mathbf{u}'(\mathbf{x}; V) \\
& \quad + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) p'(\mathbf{x}; V) + \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{n}'(\mathbf{x}; V) + \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \mathbf{t}'(\mathbf{x}; V) \\
& \quad + [\nabla J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \nabla \mathbf{u} + \nabla \nabla \mathbf{u} : \nabla_{\nabla \mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \\
& \qquad + \nabla \mathbf{n} \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \nabla \mathbf{t} : \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t})] \cdot V(0) \\
& \quad + J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p, \mathbf{n}, \mathbf{t}) (\nabla \cdot V(0) - DV(0)\mathbf{n} \cdot \mathbf{n}) \, \mathrm{d}\Gamma,
\end{aligned}$$

Test (3.21.6) with the adjoint variable $(\mathbf{v}, q)$, obtain

$$\begin{cases}
\int_\Omega D_{\mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v} + D_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \nabla \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v} + D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla \\
\quad + D_p \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) p'(\mathbf{x}; V) \cdot \mathbf{v} + D_{\nabla p} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \nabla p'(\mathbf{x}; V) \cdot \mathbf{v} \mathrm{d}\mathbf{x} \\
\qquad = \int_\Omega D_{\mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v} + D_{\nabla \mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \nabla \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v} + D_p \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) p'(\mathbf{x}; V) \cdot \mathbf{v} \mathrm{d}\mathbf{x}, \\
\int_\Omega -q \nabla \cdot \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\mathbf{x} = \int_\Omega q D_{\mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \mathbf{u}'(\mathbf{x}; V) + q D_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p) \nabla \mathbf{u}'(\mathbf{x}; V) + q D_p f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p
\end{cases}$$

Integrate by parts:

(a) Term $D_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \nabla \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v}$: Use the result for term 2 before with $\tilde{\mathbf{u}} := \mathbf{u}'(\mathbf{x}; V)$:

$$\begin{aligned}
& \int_\Omega D_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \nabla \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v} \mathrm{d}\mathbf{x} \\
= & -\int_\Omega (\nabla \cdot (\nabla_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p)) \cdot \mathbf{v}) \cdot \mathbf{u}'(\mathbf{x}; V) + (\nabla_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) : \nabla \mathbf{v}) \cdot \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\mathbf{x} \\
& + \int_\Gamma ((\nabla_{\nabla \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \cdot \mathbf{n}) \cdot \mathbf{v}) \cdot \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\Gamma.
\end{aligned}$$

(b) Term $D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \Delta \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v}$: Use the result for term 3 before with $\tilde{\mathbf{u}} := \mathbf{u}'(\mathbf{x}; V)$:

$$\begin{aligned}
& \int_\Omega D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \Delta \mathbf{u}'(\mathbf{x}; V) \cdot \mathbf{v} \mathrm{d}\mathbf{x} \\
= & \int_\Omega \mathbf{v}^\top \Delta D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{u}'(\mathbf{x}; V) + \Delta \mathbf{v}^\top D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\mathbf{x} \\
& - \int_\Gamma \mathbf{v}^\top D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \partial_{\mathbf{n}} \mathbf{u}'(\mathbf{x}; V) - \mathbf{v}^\top \partial_{\mathbf{n}} D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{u}'(\mathbf{x}; V) \\
& \qquad - \partial_{\mathbf{n}} \mathbf{v}^\top D_{\Delta \mathbf{u}} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \mathbf{u}'(\mathbf{x}; V) \mathrm{d}\Gamma.
\end{aligned}$$

(c) Term $D_{\nabla p} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \nabla p'(\mathbf{x}; V) \cdot \mathbf{v}$: Use the result for term 5 before with $\tilde{\mathbf{u}} := \mathbf{u}'(\mathbf{x}; V)$:

$$\int_\Omega D_{\nabla p} \mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, \Delta \mathbf{u}, p, \nabla p) \nabla p'(\mathbf{x}; V) \cdot \mathbf{v} \mathrm{d}\mathbf{x}$$

$$= -\int_\Omega p'(\mathbf{x};V)\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) : \nabla\mathbf{v} + p'(\mathbf{x};V)\nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p))\cdot\mathbf{v}\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}\mathrm{d}\Gamma.$$

(d) Term $D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V)\cdot\mathbf{v}$: Use the result for term 4 before with $\tilde{\mathbf{u}} := \mathbf{u}'(\mathbf{x};V)$:

$$\int_\Omega D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V)\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_\Omega (\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\cdot\mathbf{v})\cdot\mathbf{u}'(\mathbf{x};V) + (\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\mathbf{v})\cdot\mathbf{u}$$
$$+ \int_\Gamma ((\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v})\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma.$$

(e) Term $q\nabla\cdot\mathbf{u}'(\mathbf{x};V)$: Use the result for term 6 before with $\tilde{\mathbf{u}} := \mathbf{u}'(\mathbf{x};V)$:

$$\int_\Omega -q\nabla\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x} = \int_\Omega \nabla q\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x} - \int_\Gamma q\mathbf{u}'(\mathbf{x};V)\cdot\mathbf{n}\mathrm{d}\Gamma.$$

(f) Term $qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V)$: Use the result for term 7 before with $\tilde{\mathbf{u}} := \mathbf{u}'(\mathbf{x};V)$:

$$\int_\Omega qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x} = -\int_\Omega \nabla^\top q\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V) + q\left(\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))\right)\cdot\mathbf{u}$$
$$+ \int_\Gamma q\mathbf{n}^\top\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma.$$

Plug in, obtain then

$$\begin{cases}
\int_\Omega [\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v} - (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) : \nabla\mathbf{v} \\
\quad + [\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathbf{v} \\
\quad - [\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{v}]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x} \\
\quad + \int_\Omega [[D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{v} \\
\quad\quad -\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p):\nabla\mathbf{v}]\,p'(\mathbf{x};V)\mathrm{d}\mathbf{x} \\
\quad + \int_\Gamma [(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n})\cdot\mathbf{v} + \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v} \\
\quad - (\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v}]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma \\
\quad + \int_\Gamma -\mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x};V) + p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}\mathrm{d}\Gamma = 0, \\
\int_\Omega [\nabla q - q\nabla_{\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + D_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla q + q\nabla\cdot(\nabla_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x} \\
\quad - \int_\Omega qD_pf_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V)\mathrm{d}\mathbf{x} - \int_\Gamma [qn + qD_{\nabla\mathbf{u}}f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n}]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma = 0.
\end{cases}$$

Add them together, obtain

$$\int_\Omega [\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\Delta\mathbf{v} - (\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) : \nabla\mathbf{v}$$
$$+ [\nabla_{\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) + \Delta\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla_{\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,\mathbf{v}$$
$$- [\nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - \nabla\cdot(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{v}$$

$$
\begin{aligned}
&\quad +\nabla q - q\nabla_{\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + D_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla q + q\nabla\cdot(\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\mathbf{x}\\
&+\int_\Omega [[D_p\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p) - \nabla\cdot(\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)) - D_p\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\cdot\mathbf{v}\\
&\quad -\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p):\nabla\mathbf{v} - qD_p f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)]\,p'(\mathbf{x};V)\mathrm{d}\mathbf{x}\\
&+\int_\Gamma [(\nabla_{\nabla\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\cdot\mathbf{n})\cdot\mathbf{v} + \partial_{\mathbf{n}}\nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v} + \nabla_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{v}\\
&\quad -(\nabla_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n})\cdot\mathbf{v} - qn - qD_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n}]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma\\
&+\int_\Gamma -\mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x};V) + p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}\mathrm{d}\Gamma = 0.
\end{aligned}
$$

Combine this with (adj-gfld), obtain

$$
\begin{aligned}
&\int_\Omega [\nabla_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) - \nabla\cdot(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{u}'(\mathbf{x};V) + D_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V)\mathrm{d}\mathbf{x}\\
&+\int_\Gamma [-\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\mathrm{bc}} + \nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{n} + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})]\cdot\mathbf{u}'(\mathbf{x};V)\mathrm{d}\Gamma\\
&+\int_\Gamma -\mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x};V) + p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}\mathrm{d}\Gamma = 0.
\end{aligned}
$$

Combine this equality with the formula of shape derivative $dJ(\mathbf{u},p,\Omega)$, obtain:

$$
\begin{aligned}
dJ(\mathbf{u},p,\Omega;V) = &\int_\Omega \nabla\cdot(J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0))\,\mathrm{d}\mathbf{x}\\
&+\int_\Gamma \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\nabla\mathbf{u}'(\mathbf{x};V) + \partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V) + \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}\\
&\qquad + \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\mathbf{t}'(\mathbf{x};V)\\
&\qquad + [\nabla J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\nabla\mathbf{u} + \nabla\nabla\mathbf{u}:\nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\\
&\qquad\quad +\partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla p + \nabla\mathbf{n}\nabla_{\mathbf{n}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + \nabla\mathbf{t}:\nabla_{\mathbf{t}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})]\cdot V\\
&\qquad + J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\,(\nabla\cdot V(0) - DV(0)\mathbf{n}\cdot\mathbf{n}) + (\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\mathrm{bc}})\cdot\mathbf{u}'(\mathbf{x};V)\\
&\qquad + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x};V) - p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}\mathrm{d}\Gamma.
\end{aligned}
$$

To eliminate $(\mathbf{u}'(\mathbf{x};V), p(\mathbf{x};V))$ in boundary integrals, we need the explicit formula of $\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})$ (but not $\mathbf{f}_{\mathrm{bc}}(\mathbf{x})$).

2. *2nd representation of shape derivative.* Use the same technique:

$$
\begin{aligned}
&dJ(\mathbf{u},p,\Omega;V)\\
=&\int_\Omega J'_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p;V)\mathrm{d}\mathbf{x}\\
&+\int_\Gamma J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0)\cdot\mathbf{n} + J'_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t};V) + [\partial_{\mathbf{n}}(J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})) + HJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})]\,V(0)\cdot\\
=&\int_\Omega D_{\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u}'(\mathbf{x};V) + \partial_p J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V)\mathrm{d}\mathbf{x}\\
&+\int_\Gamma J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0)\cdot\mathbf{n} + D_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{u}'(\mathbf{x};V) + D_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\nabla\mathbf{u}'(\mathbf{x};V)\\
&\qquad + \partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V) + D_{\mathbf{n}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{n}'(\mathbf{x};V) + D_{\mathbf{t}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{t}'(\mathbf{x};V)\\
&\qquad + [DJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}) + D_{\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\mathbf{u} + D_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\nabla\mathbf{u} + \partial_p J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{r}
\end{aligned}
$$

$$
\begin{aligned}
&\qquad +D_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\mathbf{n}+D_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})D\mathbf{t}]\cdot\mathbf{n}V(0)\cdot\mathbf{n}+HJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})V(0)\cdot\mathbf{n}\mathrm{d}\Gamma\\
&=\int_\Omega \nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{u}'(\mathbf{x};V)+\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\mathbf{u}'(\mathbf{x};V)+\partial_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V)\mathrm{d}\mathbf{x}\\
&\quad+\int_\Gamma J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0)\cdot\mathbf{n}+\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{u}'(\mathbf{x};V)+\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\nabla\mathbf{u}'(\mathbf{x};V)\\
&\qquad+\partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V)+\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{n}'(\mathbf{x};V)+\nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\mathbf{t}'(\mathbf{x};V)\\
&\qquad+[\nabla J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\nabla\mathbf{u}+\nabla\nabla\mathbf{u}:\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\\
&\qquad\quad+\nabla\mathbf{n}\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\nabla\mathbf{t}:\nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})]\cdot\mathbf{n}V(0)\cdot\mathbf{n}+HJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})V(0)\cdot\mathbf{n}\mathrm{d}\\
&=\int_\Omega [\nabla_{\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)-\nabla\cdot(\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p))]\cdot\mathbf{u}'(\mathbf{x};V)+\partial_pJ_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)p'(\mathbf{x};V)\mathrm{d}\mathbf{x}\\
&\quad+\int_\Gamma J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0)\cdot\mathbf{n}+\mathbf{n}^\top\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{u}'(\mathbf{x};V)+\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{u}'(\mathbf{x};V)\\
&\qquad+\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\nabla\mathbf{u}'(\mathbf{x};V)+\partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V)+\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{n}'(\mathbf{x};V)\\
&\qquad+\nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\mathbf{t}'(\mathbf{x};V)\\
&\qquad+[\nabla J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\nabla\mathbf{u}+\nabla\nabla\mathbf{u}:\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\\
&\qquad\quad+\nabla\mathbf{n}\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\nabla\mathbf{t}:\nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})]\cdot\mathbf{n}V(0)\cdot\mathbf{n}+HJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})V(0)\cdot\mathbf{n}\mathrm{d}\\
&=\int_\Gamma J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)V(0)\cdot\mathbf{n}+\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\nabla\mathbf{u}'(\mathbf{x};V)+\partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})p'(\mathbf{x};V)\\
&\qquad+\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\mathbf{n}'(\mathbf{x};V)+\nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t}):\mathbf{t}'(\mathbf{x};V)\\
&\qquad+[\nabla J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\nabla_{\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\cdot\nabla\mathbf{u}+\nabla\nabla\mathbf{u}:\nabla_{\nabla\mathbf{u}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\partial_pJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\\
&\qquad\quad+\nabla\mathbf{n}\nabla_{\mathbf{n}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})+\nabla\mathbf{t}:\nabla_{\mathbf{t}}J_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})]\cdot\mathbf{n}V(0)\cdot\mathbf{n}+HJ_\Gamma(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})V(0)\cdot\mathbf{n}\\
&\qquad+(\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})\mathbf{v}_{\mathrm{bc}})\cdot\mathbf{u}'(\mathbf{x};V)+\mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x};V)\\
&\qquad-p'(\mathbf{x};V)\mathbf{n}^\top\nabla_{\nabla p}\mathbf{P}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},\Delta\mathbf{u},p,\nabla p)\mathbf{v}\mathrm{d}\Gamma.
\end{aligned}
$$

To eliminate $(\mathbf{u}'(\mathbf{x};V),p(\mathbf{x};V))$ in boundary integrals, we need the explicit formula of $\mathbf{Q}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p,\mathbf{n},\mathbf{t})$ (but not $\mathbf{f}_{\mathrm{bc}}(\mathbf{x})$).

Conclude: The 1st-order shape derivative of (cost-gfld) under the state constraint (gfld) s given by either of the following representations:

$$
\begin{aligned}
& dJ(\mathbf{u}, p, \Omega; V) \\
&= \int_\Omega \nabla \cdot (J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)V(0))\,\mathrm{d}\mathbf{x} \\
&\quad + \int_\Gamma \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla\mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})p'(\mathbf{x}; V) + \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{n}'(\mathbf{x}; V) \\
&\qquad\quad + \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \mathbf{t}'(\mathbf{x}; V) + \nabla\left(J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\right) \cdot V(0) \\
&\qquad\quad + J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\left(\nabla \cdot V(0) - DV(0)\mathbf{n} \cdot \mathbf{n}\right) + (\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\mathbf{v}_{\mathrm{bc}}) \cdot \mathbf{u}'(\mathbf{x}; V) \\
&\qquad\quad + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x}; V) - p'(\mathbf{x}; V)\mathbf{n}^\top \nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v}\,\mathrm{d}\Gamma \\
&= \int_\Omega \nabla \cdot (J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)V(0))\,\mathrm{d}\mathbf{x} \\
&\quad + \int_\Gamma \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla\mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})p'(\mathbf{x}; V) \\
&\qquad\quad + \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{n}'(\mathbf{x}; V) + \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \mathbf{t}'(\mathbf{x}; V) \\
&\qquad\quad + [\nabla J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \nabla\mathbf{u} + \nabla\nabla\mathbf{u} : \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \\
&\qquad\qquad + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\nabla p + \nabla\mathbf{n}\nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \nabla\mathbf{t} : \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})] \cdot V(0) \\
&\qquad\quad + J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\left(\nabla \cdot V(0) - DV(0)\mathbf{n} \cdot \mathbf{n}\right) + (\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\mathbf{v}_{\mathrm{bc}}) \cdot \mathbf{u}'(\mathbf{x}; V) \\
&\qquad\quad + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x}; V) - p'(\mathbf{x}; V)\mathbf{n}^\top \nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v}\,\mathrm{d}\Gamma \\
&= \int_\Gamma J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)V(0) \cdot \mathbf{n} + \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla\mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})p'(\mathbf{x}; V) \\
&\qquad\quad + \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{n}'(\mathbf{x}; V) + \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \mathbf{t}'(\mathbf{x}; V) \\
&\qquad\quad + \partial_{\mathbf{n}}\left(J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\right)V(0) \cdot \mathbf{n} + HJ_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})V(0) \cdot \mathbf{n} \\
&\qquad\quad + (\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\mathbf{v}_{\mathrm{bc}}) \cdot \mathbf{u}'(\mathbf{x}; V) + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x}; V) \\
&\qquad\quad - p'(\mathbf{x}; V)\mathbf{n}^\top \nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v}\,\mathrm{d}\Gamma \\
&= \int_\Gamma J_\Omega(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)V(0) \cdot \mathbf{n} + \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \nabla\mathbf{u}'(\mathbf{x}; V) + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})p'(\mathbf{x}; V) \\
&\qquad\quad + \nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \mathbf{n}'(\mathbf{x}; V) + \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) : \mathbf{t}'(\mathbf{x}; V) \\
&\qquad\quad + [\nabla J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \nabla_{\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) \cdot \nabla\mathbf{u} + \nabla\nabla\mathbf{u} : \nabla_{\nabla\mathbf{u}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \partial_p J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u} \\
&\qquad\qquad + \nabla\mathbf{n}\nabla_{\mathbf{n}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t}) + \nabla\mathbf{t} : \nabla_{\mathbf{t}} J_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})] \cdot \mathbf{n}V(0) \cdot \mathbf{n} + HJ_\Gamma(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})V(0) \cdot \mathbf{n} \\
&\qquad\quad + (\nabla_{\mathbf{u}}\mathbf{Q}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p, \mathbf{n}, \mathbf{t})\mathbf{v}_{\mathrm{bc}}) \cdot \mathbf{u}'(\mathbf{x}; V) + \mathbf{v}^\top D_{\Delta\mathbf{u}}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\partial_{\mathbf{n}}\mathbf{u}'(\mathbf{x}; V) \\
&\qquad\quad - p'(\mathbf{x}; V)\mathbf{n}^\top \nabla_{\nabla p}\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, \Delta\mathbf{u}, p, \nabla p)\mathbf{v}\,\mathrm{d}\Gamma
\end{aligned}
$$

3.22 Stationary incompressible viscous Navier-Stokes equations

Consider the following stationary incompressible viscous Navier-Stokes equations:

$$
\begin{cases}
-\nabla \cdot (\nu(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p)\nabla\mathbf{u}) + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \mathbf{f}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) & \text{in } \Omega, \\
\nabla \cdot \mathbf{u} = f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u}, p) & \text{in } \Omega.
\end{cases}
\tag{NS}
$$

3.23 Weak formulations for stationary incompressible viscous Navier-Stokes equations

Test both sides of the 1st equation of (**??**) with a test function $\mathbf{v}$ and those of the 2nd one with a test function q over Ω:

$$\begin{cases} \displaystyle\int_\Omega -\nabla\cdot(\nu(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u})\cdot\mathbf{v} + (\mathbf{u}\cdot\nabla)\,\mathbf{u}\cdot\mathbf{v} + \nabla p\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v}\mathrm{d}\mathbf{x}, \\ \displaystyle\int_\Omega q\nabla\cdot\mathbf{u}\mathrm{d}\mathbf{x} = \int_\Omega q f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x}. \end{cases} \tag{test-gsincNS}$$

Apply (ibp-mat2) for the 1st term in the l.h.s. of the 1st equation of (test-gsincNS):

$$\int_\Omega -\nabla\cdot(\nu(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u})\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \nu(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u} : \nabla\mathbf{v}\mathrm{d}\mathbf{x} - \int_\Gamma \nu(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n}^\top\nabla\mathbf{u}\mathbf{v}\mathrm{d}\Gamma.$$

Apply (ibp) for the 3rd term in the l.h.s. of the 1st equation of (test-gsincNS):

$$\int_\Omega \nabla p\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_\Omega p\nabla\cdot\mathbf{v}\mathrm{d}\mathbf{x} + \int_\Gamma p\mathbf{v}\cdot\mathbf{n}\mathrm{d}\Gamma.$$

Keep the 2nd equation of (test-gsincNS), then it becomes

$$\begin{cases} \displaystyle\int_\Omega \nu(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\mathbf{u} : \nabla\mathbf{v} + (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v} - p\nabla\cdot\mathbf{v} - \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\cdot\mathbf{v}\mathrm{d}\mathbf{x} + \int_\Gamma p\mathbf{v}\cdot\mathbf{n} - \nu(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathbf{n}^\top\nabla\mathbf{u}\mathbf{v}\mathrm{d}\Gamma = 0 \\ \displaystyle\int_\Omega q\nabla\cdot\mathbf{u} - q f_{\rm div}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x} = 0 \end{cases} \tag{wf-gsincNS}$$

3.24 A general cost functionals & its associated optimization problem

The optimization problem associated with the cost functional (cost-gfld) can be formulated as follows:

Find Ω over a class of admissible domain $\mathcal{O}_{\rm ad}$ s.t. the cost functional (cost-gfld) is minimized subject to (**??**), i.e.:

$$\min_{\Omega\in\mathcal{O}_{\rm ad}} J(\mathbf{u},p,\Omega) \text{ s.t. } (\mathbf{u},p) \text{ solves } (\mathbf{??}). \tag{opt-gsincNS}$$

Chapter 4

Shape Optimization for General Conservation Laws

4.1 General conservation equation

We consider the following general conservation equation in differential form (see, e.g., Ferziger, Perić, and Street, 2020, Moukalled, Mangani, and Darwish, 2016, Sect. 3.7):

$$\partial_t(\rho\phi) + \nabla \cdot (\rho \mathbf{u}\phi) = \nabla \cdot (\Gamma^\phi \nabla \phi) + q^\phi, \tag{gcl}$$

which may be rewritten as

$$\partial_t(\rho\phi) + \nabla \cdot \mathbf{J}^\phi = q^\phi,$$

where the *total flux* $\mathbf{J}^\phi$ is the sum of the *convective* and *diffusive fluxes* given by

$$\mathbf{J}^\phi \coloneqq \mathbf{J}^\phi_{\text{conv}} + \mathbf{J}^\phi_{\text{diff}}, \text{ where } \mathbf{J}^\phi_{\text{conv}} \coloneqq \rho\mathbf{u}\phi,\ \mathbf{J}^\phi_{\text{diff}} \coloneqq -\Gamma^\phi \nabla\phi.$$

The integral form of the *generic conservation equation* (see, e.g., Ferziger, Perić, and Street, 2020):

$$\partial_t \int_V \rho\phi \mathrm{d}V + \int_S \rho\phi\mathbf{v} \cdot \mathbf{n} \mathrm{d}S = \int_S \Gamma\nabla\phi \cdot \mathbf{n} \mathrm{d}S + \int_V q_\phi \mathrm{d}V,$$

where q_ϕ is the source or sink of ϕ.

The coordinate-free vector form of this equation is:

$$\partial_t(\rho\phi) + \nabla \cdot (\rho\phi\mathbf{v}) = \nabla \cdot (\Gamma\nabla\phi) + q_\phi.$$

Special features of NSEs will be described afterwards as an extension of the methods for the generic equation.

We also consider the steady-state/stationary form of (gcl):

$$\nabla \cdot (\rho\mathbf{u}\phi) = \nabla \cdot (\Gamma^\phi \nabla\phi) + q^\phi. \tag{sgcl}$$

Let $(\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible finite volume mesh defined in Definition B.4.4. Integrating (sgcl) over an element $K \in \mathcal{T}$ yields

$$\int_K \nabla \cdot (\rho\mathbf{u}\phi) \mathrm{d}\mathbf{x} = \int_K \nabla \cdot (\Gamma^\phi \nabla\phi) \mathrm{d}\mathbf{x} + \int_K q^\phi \mathrm{d}\mathbf{x}. \tag{4.1.1}$$

Applying (div) with $\Omega = K$, $\boldsymbol{\phi} = \rho\mathbf{u}\phi$ and $\boldsymbol{\phi} = \Gamma^\phi \nabla\phi$ yields

$$\int_K \nabla \cdot (\rho\mathbf{u}\phi)\mathrm{d}\mathbf{x} = \int_{\partial K} \rho\phi\mathbf{u}\cdot\mathbf{n}\mathrm{d}\partial K = \int_{\partial K} \rho\phi\mathbf{u}_\mathbf{n}\mathrm{d}\partial K,$$
$$\int_K \nabla \cdot (\Gamma^\phi\nabla\phi)\mathrm{d}\mathbf{x} = \int_{\partial K} \Gamma^\phi\nabla\phi\cdot\mathbf{n}\mathrm{d}\partial K = \int_{\partial K} \Gamma^\phi\partial_\mathbf{n}\phi\mathrm{d}\partial K.$$

Then (4.1.1) becomes

$$\int_{\partial K} \rho\phi\mathbf{u}\cdot\mathbf{n}\mathrm{d}\partial K = \int_{\partial K} \Gamma^\phi\nabla\phi\cdot\mathbf{n}\mathrm{d}\partial K + \int_K q^\phi \mathrm{d}\mathbf{x}.$$

Replacing the surface integral over the cell K by a summation of the flux terms over the edges/faces of element K, the surface integrals of the convection-, diffusion-, and total fluxes become

$$\int_{\partial K} \mathbf{J}^\phi_{\text{conv}}\cdot\mathbf{n}\mathrm{d}\partial K = \int_{\partial K} \rho\phi\mathbf{u}\cdot\mathbf{n}\mathrm{d}\partial K = \sum_{\sigma\in\mathcal{E}_K}\int_\sigma \rho\phi\mathbf{u}\cdot\mathbf{n}\mathrm{d}\sigma,$$
$$\int_{\partial K} \mathbf{J}^\phi_{\text{diff}}\cdot\mathbf{n}\mathrm{d}\partial K = \int_{\partial K} \Gamma^\phi\nabla\phi\cdot\mathbf{n}\mathrm{d}\partial K = \sum_{\sigma\in\mathcal{E}_K}\int_\sigma \Gamma^\phi\nabla\phi\cdot\mathbf{n}\mathrm{d}\sigma,$$
$$\int_{\partial K} \mathbf{J}^\phi\cdot\mathbf{n}\mathrm{d}\partial K = \int_{\partial K} (\mathbf{J}^\phi_{\text{conv}} + \mathbf{J}^\phi_{\text{diff}})\cdot\mathbf{n}\mathrm{d}\partial K = \sum_{\sigma\in\mathcal{E}_K}\int_\sigma (\rho\phi\mathbf{u} + \Gamma^\phi\nabla\phi)\cdot\mathbf{n}\mathrm{d}\sigma.$$

Then some appropriate *numerical quadratures/numerical integration formulas* can be used to approximate these surface integrals and also the volume integral for q^ϕ (see, e.g., Isaacson and Keller, 1994, Chap. 7).

Part II

Shape Optimization for Large Eddy Simulation Turbulence Models

In this part, we consider the following governing equations (see, e.g., John, 2004)

$$\begin{cases} \mathbf{w}_t - \nabla\cdot((2\nu+\nu_{\mathrm{t}})\boldsymbol{\varepsilon}(\mathbf{w})) + (\mathbf{w}\nabla)\mathbf{w} + \nabla r + \nabla\cdot\dfrac{\delta^2}{2\gamma}\left(A(\nabla\mathbf{w}\otimes\nabla\mathbf{w})\right) = \mathbf{f}, & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\mathbf{w} = 0, & \text{in } [0,T]\times\Omega. \end{cases} \tag{4.1.2}$$

Chapter 5

Shape Optimization for Smagorinsky Turbulence Model

In B. Mohammadi and O. Pironneau, 1994: "Mathematically the Smagorinsky system is better than Navier-Stokes' because there is existence, uniqueness and regularity even in 3D (Lions[1968])".

5.1 Notation

Let $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, a bounded domain with Lipschitz boundary Γ given as $\Gamma := \Gamma_{\text{in}} \cup \Gamma_{\text{wall}} \cup \Gamma_{\text{out}}$ and $T > 0$. Denote by

$$\varepsilon(\mathbf{v}) := \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^\top)$$

the symmetrized gradient of $\mathbf{v} \in H^1(\Omega)$.

The Banach space

$$W^{1,3}_{0,\text{div}}(\Omega) = \{\mathbf{v} \in W^{1,3}(\Omega); \mathbf{v}|_{\partial\Omega} = \mathbf{0},\ \nabla \cdot \mathbf{v} = 0 \text{ in } \Omega\}$$

is equipped with the same norm as $W^{1,3}_0(\Omega)$. Let

$$V = H^1(0, T; L^2(\Omega)) \cap L^3(0, T; W^{1,3}_{0,\text{div}}(\Omega))$$

equipped with

$$\|\mathbf{v}\|_V = \|\nabla \mathbf{v}\|_{L^3(0,T;L^3(\Omega))} + \|\mathbf{v}_t\|_{L^2(0,T;L^2(\Omega))}.$$

5.2 Smagorinsky turbulence model with homogeneous boundary conditions

We consider the following instationary NSEs:

$$\begin{cases} \mathbf{u}_t - \nu \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \mathbf{f} & \text{in } (0, T] \times \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \text{in } [0, T] \times \Omega, \\ \mathbf{u}(0, \cdot) = \mathbf{u}_0 & \text{in } \Omega, \\ \mathbf{u} = \mathbf{0} & \text{on } [0, T] \times \Gamma, \\ \displaystyle\int_\Omega p \mathrm{d}x = 0 & \text{in } (0, T] \end{cases} \tag{5.2.1}$$

The initial flow field $\mathbf{u}_0(x)$ is also divergence-free, i.e. $\nabla \cdot \mathbf{u}_0 = 0$ in Ω.

We define the Smagorinsky turbulence models

$$\begin{cases} \mathbf{w}_t - \nabla \cdot ((\nu + \nu_S \|\nabla \mathbf{w}\|_F)\nabla \mathbf{w}) + (\mathbf{w}\cdot\nabla)\mathbf{w} + \nabla r = \mathbf{f} & \text{in } (0,T]\times\Omega, \\ \nabla\cdot\mathbf{w} = 0 & \text{in } [0,T]\times\Omega, \\ \mathbf{w} = \mathbf{0} & \text{on } [0,T]\times\Gamma, \\ \mathbf{w}(0,\cdot) = \mathbf{w}_0 & \text{in } \Omega, \\ \int_\Omega r \mathrm{d}x = 0 & \text{in } (0,T], \end{cases} \tag{5.2.2}$$

with $\nu_S > 0$, $\mathbf{f} \in L^2(0,T;L^2(\Omega))$ and $T \in (0,\infty)$.

5.2.1 Weak formulation

The weak formulation of (5.2.2) reads:

Find $\mathbf{w} \in V$ s.t. $\mathbf{w}(0,x) = \mathbf{w}_0 \in W^{1,3}_{0,\mathrm{div}}(\Omega)$ and for all $\mathbf{v} \in V$

$$\int_0^T \mathbf{w}_t \cdot \mathbf{v} + (\mathbf{w}\cdot\nabla)\mathbf{w}\cdot\mathbf{v} + (\nu + \nu_S\|\nabla\mathbf{w}\|_F)\nabla\mathbf{w}\cdot\nabla\mathbf{v}\mathrm{d}t = \int_0^T \mathbf{f}\cdot\mathbf{v}\mathrm{d}t. \tag{5.2.3}$$

Definition 5.2.1. *A function $\mathbf{w} \in V$ satisfying (5.2.3) is called a* weak solution *of the Smagorinsky model.*

See John, 2004, Lemmas 6.1, 6.2 and 6.3, pp. 75–76:

Lemma 5.2.1. *Assume that (5.2.2) has a sufficiently smooth solution $(\mathbf{w}, r)$. Then, for $T > 0$, this solution satisfies*

$$\|\mathbf{w}(T)\|_{L^2(\Omega)} \le \|\mathbf{w}_0\|_{L^2(\Omega)} + \int_0^T \|\mathbf{f}(t,x)\|_{L^2(\Omega)}\mathrm{d}t,$$

$$\|\mathbf{w}(T,x)\|^2_{L^2(\Omega)} + 2\int_0^T (\nu+\nu_S\|\nabla\mathbf{w}\|_F)\nabla\mathbf{w}\cdot\nabla\mathbf{w}\mathrm{d}t \le 2\|\mathbf{w}_0\|^2_{L^2(\Omega)} + 3\left(\int_0^T \|\mathbf{f}(t)\|_{L^2(\Omega)}\mathrm{d}t\right)^2 = c_1(T),$$

$$\|\nabla\mathbf{w}(T)\|^3_{L^3(\Omega)} + \frac{3}{2\nu_S}\int_0^T \|\mathbf{w}_t\|^2_{L^2(\Omega)}\mathrm{d}t \le c_2(T).$$

The nonlinear viscous operator $\mathbf{A} : L^3(\Omega) \to L^{3/2}(\Omega)$ with

$$\mathbf{A}(\nabla\mathbf{w}^n) = (\nu + \nu_S\|\nabla\mathbf{w}^n\|_F)\nabla\mathbf{w}^n.$$

See John, 2004, Lemma 6.9, pp. 85:

Lemma 5.2.2. *For arbitrary functions $\mathbf{w}', \mathbf{w}'' \in W^{1,3}(\Omega)$ holds the estimate*

$$\int_\Omega (\mathbf{A}(\nabla\mathbf{w}') - A(\nabla\mathbf{w}'')) : (\nabla\mathbf{w}' - \nabla\mathbf{w}'')\mathrm{d}x \ge \nu\|\nabla\mathbf{w}' - \nabla\mathbf{w}''\|^2_{L^2(\Omega)}. \tag{5.2.4}$$

Moreover, the Smagorinsky term defines a monotone operator from $L^3(\Omega)$ into $L^{3/2}(\Omega)$.

See John, 2004, Theorem 6.12, p. 89:

Theorem 5.2.1 (Existence of a weak solution)**.** *Problem (5.2.3) possesses at least one solution $\mathbf{w} \in V$ for arbitrary $\mathbf{f} \in L^2(0,T;L^2(\Omega))$ and $\mathbf{w}_0 \in W^{1,3}_{0,\mathrm{div}}(\Omega)$.*

5.3 Smagorinsky turbulence model with mixed boundary conditions

We consider the following instationary NSEs:

$$\begin{cases} \mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f} & \text{in } (0,T]\times\Omega, \\ \nabla\cdot\mathbf{u} = 0 & \text{in } [0,T]\times\Omega, \\ \mathbf{u}(0,\cdot) = \mathbf{u}_0 & \text{in } \Omega, \\ \mathbf{u} = \mathbf{f}_{\text{in}} & \text{on } [0,T]\times\Gamma_{\text{in}}, \\ \mathbf{u} = \mathbf{0} & \text{on } [0,T]\times\Gamma_{\text{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{u} + p\mathbf{n} = \mathbf{0} & \text{on } [0,T]\times\Gamma_{\text{out}}. \end{cases} \tag{5.3.1}$$

We define the Smagorinsky turbulence models

$$\begin{cases} \mathbf{w}_t - \nabla\cdot((2\nu+\nu_t)\varepsilon(\mathbf{w})) + (\mathbf{w}\cdot\nabla)\mathbf{w} + \nabla r = \mathbf{f} & \text{in } (0,T]\times\Omega, \\ \nabla\cdot\mathbf{w} = 0 & \text{in } [0,T]\times\Omega, \\ \mathbf{w}(0,\cdot) = \mathbf{w}_0 & \text{in } \Omega, \\ \mathbf{w} = \mathbf{f}_{\text{in}} & \text{on } [0,T]\times\Gamma_{\text{in}}, \\ \mathbf{w} = \mathbf{0} & \text{on } [0,T]\times\Gamma_{\text{wall}}, \\ -\nu\partial_{\mathbf{n}}\mathbf{w} + r\mathbf{n} = \mathbf{0} & \text{on } [0,T]\times\Gamma_{\text{out}}, \end{cases} \tag{5.3.2}$$

where $\nu_t = \nu_S\|\nabla\mathbf{w}\|_{\mathrm{F}}$

Part III

Shape Optimization for Reynolds-Averaged Navier-Stokes Equations

Chapter 6

Shape Optimization for k-ϵ Turbulence Model

6.1 Derivation of k-ϵ turbulence model

Reynolds hypothesis is that the turbulence in the flow is a local function of $2\boldsymbol{\varepsilon}(\overline{\mathbf{u}}) = \nabla\overline{\mathbf{u}} + (\nabla\overline{\mathbf{u}})^\top$, i.e., $R(t,\mathbf{x}) = R(2\boldsymbol{\varepsilon}(\overline{\mathbf{u}}(t,\mathbf{x})))$ (see, e.g., B. Mohammadi and O. Pironneau, 1994; Bijan Mohammadi and Olivier Pironneau, 2010).

Denote by k the kinetic energy of small scales and ϵ their rate of viscous energy dissipation:

$$k \coloneqq \frac{1}{2}\overline{|\mathbf{u}'|^2},\ \epsilon \coloneqq 2\nu\overline{\|\boldsymbol{\varepsilon}(\mathbf{u}')\|_{\mathrm{F}}^2} = \frac{\nu}{2}\overline{\|\nabla\mathbf{u}' + (\nabla\mathbf{u}')^\top\|_{\mathrm{F}}^2}, \tag{6.1.1}$$

where $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius norm of a matrix.

For 2D mean flows and for some $\alpha(t,\mathbf{x})$,

$$R = 2\nu_{\mathrm{t}}\boldsymbol{\varepsilon}(\overline{\mathbf{u}}) + \alpha I,\ \nu_{\mathrm{t}} = c_\mu\frac{k^2}{\epsilon},$$

and k and ϵ are modeled by

$$\begin{cases} \partial_t k + \overline{\mathbf{u}}\cdot\nabla k - 2c_\mu\dfrac{k^2}{\epsilon}\|\boldsymbol{\varepsilon}(\overline{\mathbf{u}})\|_{\mathrm{F}}^2 - \nabla\cdot\left(c_\mu\dfrac{k^2}{\epsilon}\nabla k\right) + \epsilon = 0, \\ \partial_t\epsilon + \overline{\mathbf{u}}\cdot\nabla\epsilon - 2c_1 k\|\boldsymbol{\varepsilon}(\overline{\mathbf{u}})\|_{\mathrm{F}}^2 - \nabla\cdot\left(c_\epsilon\dfrac{k^2}{\epsilon}\nabla\epsilon\right) + c_2\dfrac{\epsilon^2}{k} = 0, \end{cases} \tag{6.1.2}$$

with $c_\mu = 0.09$, $c_1 = 0.126$, $c_2 = 1.92$, $c_\epsilon = 0.07$.

Given a filter $\langle\cdot\rangle$, the incompressible Reynolds averaged NSEs for the *mean flow* $\overline{\mathbf{u}}$ and *mean pressure* $\overline{p}$ are

$$\begin{cases} \overline{\mathbf{u}}_t - \nu\Delta\overline{\mathbf{u}} + (\overline{\mathbf{u}}\cdot\nabla)\overline{\mathbf{u}} + \nabla\overline{p} - \nabla\cdot R(k,\varepsilon,\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top) = 0 & \text{in } (0,T)\times\Omega, \\ \nabla\cdot\overline{\mathbf{u}} = 0 & \text{in } (0,T)\times\Omega, \end{cases} \tag{6.1.3}$$

where $R_{ij} = -\langle u_i u_j\rangle$ is the Reynolds tensor. The kinetic energy of the turbulence k and the rate of dissipation of turbulent energy ε are defined by

$$k = \frac{1}{2}\langle|\mathbf{u}'|^2\rangle,\ \varepsilon = \frac{\nu}{2}\langle|\nabla\mathbf{u}' + \nabla\mathbf{u}'^\top|^2\rangle, \tag{6.1.4}$$

then R, k, ϵ are modeled in terms of the mean flow $\overline{\mathbf{u}}$ by

$$R = -\frac{2}{3}kI + \left(\nu + c_\mu \frac{k^2}{\varepsilon}\right)(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top) \text{ in } (0,T)\times\Omega, \tag{6.1.5}$$

$$k_t + (\overline{\mathbf{u}}\cdot\nabla)k - \nabla\cdot\left(c_\mu\frac{k^2}{\varepsilon}\nabla k\right) - \frac{c_\mu}{2}\frac{k^2}{\varepsilon}|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + \varepsilon = 0 \text{ in } (0,T)\times\Omega, \tag{6.1.6}$$

$$\varepsilon_t + (\overline{\mathbf{u}}\cdot\nabla)\varepsilon - \nabla\cdot\left(c_\varepsilon\frac{k^2}{\varepsilon}\nabla\varepsilon\right) - \frac{c_1}{2}k|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + c_2\frac{\varepsilon^2}{k} = 0 \text{ in } (0,T)\times\Omega, \tag{6.1.7}$$

with $c_\mu = 0.09$, $c_1 = 0.126$, $c_2 = 1.92$, $c_\varepsilon = 0.07$.

Let $\nu_{\mathrm{t}} = c_\mu\frac{k^2}{\varepsilon}$, then the k-ε and the NSEs can be rewritten as

$$k_t + (\overline{\mathbf{u}}\cdot\nabla)k - \nabla\cdot(\nu_{\mathrm{t}}\nabla k) - \frac{c_\mu}{2}\frac{k^2}{\varepsilon}|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + \varepsilon = 0, \tag{6.1.8}$$

$$\varepsilon_t + (\overline{\mathbf{u}}\cdot\nabla)\varepsilon - \nabla\cdot\left(\frac{c_\varepsilon}{c_\mu}\nu_{\mathrm{t}}\nabla\varepsilon\right) - \frac{c_1}{2}k|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + c_2\frac{\varepsilon^2}{k} = 0, \tag{6.1.9}$$

$$\overline{\mathbf{u}}_t + (\overline{\mathbf{u}}\cdot\nabla)\overline{\mathbf{u}} - \nabla\cdot\left((\nu+\nu_{\mathrm{t}})(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top)\right) + \nabla\left(\overline{p} + \frac{2}{3}k\right) = \overline{\mathbf{f}}, \tag{6.1.10}$$

$$\nabla\cdot\overline{\mathbf{u}} = 0. \tag{6.1.11}$$

6.2 Cost functional

6.3 Formal Lagrangian

We consider the following Lagrange function: [add ICs and BCs later]

$$\begin{aligned}
&\mathcal{L}(\overline{\mathbf{u}}, \overline{p}, k, \varepsilon, \Omega, \mathbf{v}, q, r, \eta) := J_{12}^{\epsilon,\gamma}(\overline{\mathbf{u}}, \overline{p}, \Omega)\\
&- \int_0^T\int_\Omega \mathbf{v}\cdot\left(\overline{\mathbf{u}}_t + (\overline{\mathbf{u}}\cdot\nabla)\overline{\mathbf{u}} - \nabla\cdot\left(\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top)\right) + \nabla\left(\overline{p} + \frac{2}{3}k\right) - \overline{\mathbf{f}}\right) - q\nabla\cdot\overline{\mathbf{u}}\,\mathrm{d}x\mathrm{d}t\\
&- \int_0^T\int_\Omega r\left(k_t + (\overline{\mathbf{u}}\cdot\nabla)k - \nabla\cdot\left(c_\mu\frac{k^2}{\varepsilon}\nabla k\right) - \frac{c_\mu}{2}\frac{k^2}{\varepsilon}|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + \varepsilon\right)\mathrm{d}x\mathrm{d}t\\
&- \int_0^T\int_\Omega \eta\left(\varepsilon_t + (\overline{\mathbf{u}}\cdot\nabla)\varepsilon - \nabla\cdot\left(c_\varepsilon\frac{k^2}{\varepsilon}\nabla\varepsilon\right) - \frac{c_1}{2}k|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + c_2\frac{\varepsilon^2}{k}\right)\mathrm{d}x\mathrm{d}t,
\end{aligned}$$

where $\mathbf{v}, q, r, \eta$ are Lagrange multipliers.

Choose the Lagrange multiplier $(\mathbf{v}, q, r, \eta)$ such that the variation with respect to the state variables vanishes identically, i.e.,

$$\partial_{\overline{\mathbf{u}}}\mathcal{L}\cdot\delta\overline{\mathbf{u}} + \partial_{\overline{p}}\mathcal{L}\delta\overline{p} + \partial_k\mathcal{L}\delta k + \partial_\varepsilon\mathcal{L}\delta\varepsilon = 0.$$

Note that

$$|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 = \left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right) : \left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right) = 2\left(\nabla\overline{\mathbf{u}} : \nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}} : \nabla\overline{\mathbf{u}}^\top\right),$$

hence

$$\partial_{\overline{\mathbf{u}}}\left(|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2\right)\delta\overline{\mathbf{u}} = 2\left(\nabla\delta\overline{\mathbf{u}} : \nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}} : \nabla\delta\overline{\mathbf{u}} + \nabla\delta\overline{\mathbf{u}} : \nabla\overline{\mathbf{u}}^\top + \nabla\overline{\mathbf{u}} : \nabla\delta\overline{\mathbf{u}}^\top\right)$$

$$= 2\left(2\nabla\overline{\mathbf{u}} : \nabla\delta\overline{\mathbf{u}} + 2\nabla\overline{\mathbf{u}}^\top : \nabla\delta\overline{\mathbf{u}}\right) = 4\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right) : \nabla\delta\overline{\mathbf{u}}.$$

Then (**??**) reads as

$$\begin{aligned}
&\partial_{\overline{\mathbf{u}}} J_{12}^{\epsilon,\gamma}(\overline{\mathbf{u}}, \overline{p}, \Omega)\cdot\delta\overline{\mathbf{u}} + \partial_{\overline{p}} J_{12}^{\epsilon,\gamma}(\overline{\mathbf{u}}, \overline{p}, \Omega)\delta\overline{p} \\
&- \int_0^T \int_\Omega \mathbf{v}\cdot\left(\delta\overline{\mathbf{u}}_t + (\delta\overline{\mathbf{u}}\cdot\nabla)\overline{\mathbf{u}} + (\overline{\mathbf{u}}\cdot\nabla)\delta\overline{\mathbf{u}} - \nabla\cdot\left(\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\left(\nabla\delta\overline{\mathbf{u}} + \nabla\delta\overline{\mathbf{u}}^\top\right)\right)\right) - q\nabla\cdot\delta\overline{\mathbf{u}}\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega r\left((\delta\overline{\mathbf{u}}\cdot\nabla)k - 2c_\mu\frac{k^2}{\varepsilon}\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right) : \nabla\delta\overline{\mathbf{u}}\right)\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega \eta\left((\delta\overline{\mathbf{u}}\cdot\nabla)\varepsilon - 2c_1k\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right) : \nabla\delta\overline{\mathbf{u}}\right)\mathrm{d}x\mathrm{d}t - \int_0^T \int_\Omega \mathbf{v}\cdot\nabla\delta\overline{p}\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega \mathbf{v}\cdot\left(-\nabla\cdot\left(2c_\mu\frac{k\delta k}{\varepsilon}\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right)\right) + \frac{2}{3}\nabla\delta k\right)\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega r\left(\delta k_t + (\overline{\mathbf{u}}\cdot\nabla)\delta k - \nabla\cdot\left(2c_\mu\frac{k\delta k}{\varepsilon}\nabla k + c_\mu\frac{k^2}{\varepsilon}\nabla\delta k\right) - c_\mu\frac{k\delta k}{\varepsilon}|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2\right)\mathrm{d}x\mathrm{d}t \\
&+ \int_0^T \int_\Omega \eta\left(\nabla\cdot\left(2c_\varepsilon\frac{k\delta k}{\varepsilon}\nabla\varepsilon\right) + \frac{c_1}{2}\delta k|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + c_2\frac{\varepsilon^2\delta k}{k^2}\right)\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega \mathbf{v}\cdot\left(\nabla\cdot\left(c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right)\right)\right)\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega r\left(\nabla\cdot\left(c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\nabla k\right) + \frac{c_\mu}{2}\frac{k^2\delta\varepsilon}{\varepsilon^2}|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top|^2 + \delta\varepsilon\right)\mathrm{d}x\mathrm{d}t \\
&- \int_0^T \int_\Omega \eta\left(\delta\varepsilon_t + (\overline{\mathbf{u}}\cdot\nabla)\delta\varepsilon - \nabla\cdot\left(-c_\varepsilon\frac{k^2\delta\varepsilon}{\varepsilon^2}\nabla\varepsilon + c_\varepsilon\frac{k^2}{\varepsilon}\nabla\delta\varepsilon\right) + 2c_2\frac{\varepsilon\delta\varepsilon}{k}\right)\mathrm{d}x\mathrm{d}t.
\end{aligned}$$

We integrate by parts all the terms which involve the derivative of directions: the term involving time derivative:

$$-\int_0^T \int_\Omega \mathbf{v}\cdot\delta\overline{\mathbf{u}}_t\mathrm{d}x\mathrm{d}t = -\int_\Omega \mathbf{v}(T)\cdot\delta\overline{\mathbf{u}}(T) - \mathbf{v}(0)\cdot\delta\overline{\mathbf{u}}(0)\mathrm{d}x + \int_0^T \int_\Omega \mathbf{v}_t\cdot\delta\overline{\mathbf{u}}\mathrm{d}x\mathrm{d}t,$$

the term produced by the nonlinear term $(\overline{\mathbf{u}}\cdot\nabla)\overline{\mathbf{u}}$:

$$-\int_\Omega \mathbf{v}\cdot((\overline{\mathbf{u}}\cdot\nabla)\delta\overline{\mathbf{u}})\mathrm{d}x = -\int_\Gamma (\overline{\mathbf{u}}\cdot\mathbf{n})(\mathbf{v}\cdot\delta\overline{\mathbf{u}})\mathrm{d}s + \int_\Omega \left[(\overline{\mathbf{u}}\cdot\nabla)\mathbf{v}\cdot\delta\overline{\mathbf{u}} + \nabla\cdot\overline{\mathbf{u}}(\mathbf{v}\cdot\delta\overline{\mathbf{u}})\right]\mathrm{d}x = -\int_\Gamma (\overline{\mathbf{u}}\cdot\mathbf{n})(\mathbf{v}\cdot\delta\overline{\mathbf{u}})\mathrm{d}s + \int_\Omega (\ldots$$

Second-order term. Since

$$\begin{aligned}
&\mathbf{v}\cdot\left(\nabla\cdot\left(\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\left(\nabla\delta\overline{\mathbf{u}} + \nabla\delta\overline{\mathbf{u}}^\top\right)\right)\right) \\
&= \mathbf{v}\cdot\left(\nabla\cdot\left(\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\left(\partial_{x_i}\delta\overline{u}_j + \partial_{x_j}\delta\overline{u}_i\right)_{i,j=1}^d\right)\right) \\
&= \mathbf{v}\cdot\left(\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\left(\sum_{j=1}^d \partial_{x_ix_j}\delta\overline{u}_j + \partial_{x_j}^2\delta\overline{u}_i\right)_{i=1}^d + \left(\sum_{j=1}^d \left(\partial_{x_i}\delta\overline{u}_j + \partial_{x_j}\delta\overline{u}_i\right)c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\right)_{i=1}^d\right) \\
&= \sum_{i=1}^d \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)v_i\sum_{j=1}^d \left(\partial_{x_ix_j}\delta\overline{u}_j + \partial_{x_j}^2\delta\overline{u}_i\right) + v_i\sum_{j=1}^d \left(\partial_{x_i}\delta\overline{u}_j + \partial_{x_j}\delta\overline{u}_i\right)c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)
\end{aligned}$$

$$= \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu \frac{k^2}{\varepsilon}\right) v_i \left(\partial_{x_i x_j}\delta\overline{u}_j + \partial_{x_j}^2 \delta\overline{u}_i\right) + c_\mu v_i \left(\partial_{x_i}\delta\overline{u}_j + \partial_{x_j}\delta\overline{u}_i\right)\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right),$$

hence

$$\begin{aligned}&\int_\Omega \mathbf{v}\cdot\left(\nabla\cdot\left(\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\left(\nabla\delta\overline{\mathbf{u}} + \nabla\delta\overline{\mathbf{u}}^\top\right)\right)\right)\mathrm{d}x \\ &= \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu \frac{k^2}{\varepsilon}\right) v_i \left(\partial_{x_i x_j}\delta\overline{u}_j + \partial_{x_j}^2 \delta\overline{u}_i\right) + c_\mu v_i \left(\partial_{x_i}\delta\overline{u}_j + \partial_{x_j}\delta\overline{u}_i\right)\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\mathrm{d}x,\end{aligned}$$

We integrate by part each term:

$$\begin{aligned}&\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right) v_i \partial_{x_i x_j}\delta\overline{u}_j \mathrm{d}x \\
=&\ \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right) v_i\partial_{x_i}\delta\overline{u}_j n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\partial_{x_i}\delta\overline{u}_j\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i\right)\mathrm{d}x \\
=&\ \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right) v_i\partial_{x_i}\delta\overline{u}_j n_j \mathrm{d}s - \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d}\delta\overline{u}_j\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i\right)n_i\mathrm{d}s \\
&+ \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\delta\overline{u}_j\left(c_\mu\partial_{x_i x_j}\left(\frac{k^2}{\varepsilon}\right)v_i + c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_i}v_i + c_\mu\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_i x_j}v_i\right)\mathrm{d}x,\end{aligned}$$

$$\begin{aligned}&\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right) v_i \partial_{x_j}^2\delta\overline{u}_i \mathrm{d}x \\
=&\ \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right) v_i\partial_{x_j}\delta\overline{u}_i n_j \mathrm{d}s - \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\partial_{x_j}\delta\overline{u}_i\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i\right)\mathrm{d}x \\
=&\ \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right) v_i\partial_{x_j}\delta\overline{u}_i n_j \mathrm{d}s - \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d}\delta\overline{u}_i\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i\right)n_j\mathrm{d}s \\
&+ \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\delta\overline{u}_i\left(c_\mu\partial_{x_j}^2\left(\frac{k^2}{\varepsilon}\right)v_i + c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i + c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}^2 v_i\right)\mathrm{d}x,\end{aligned}$$

$$\begin{aligned}&\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} c_\mu v_i\partial_{x_i}\delta\overline{u}_j\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\mathrm{d}x \\
=&\ \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d} c_\mu v_i\delta\overline{u}_j\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)n_i\mathrm{d}s - \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\delta\overline{u}_j\left(c_\mu\partial_{x_i}v_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right) + c_\mu v_i\partial_{x_i x_j}\left(\frac{k^2}{\varepsilon}\right)\right)\mathrm{d}x,\end{aligned}$$

$$\begin{aligned}&\int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d} c_\mu v_i\partial_{x_j}\delta\overline{u}_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\mathrm{d}x \\
=&\ \int_\Gamma \sum_{i=1}^{d}\sum_{j=1}^{d} c_\mu v_i\delta\overline{u}_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)n_j\mathrm{d}s - \int_\Omega \sum_{i=1}^{d}\sum_{j=1}^{d}\delta\overline{u}_i\left(c_\mu\partial_{x_j}v_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right) + c_\mu v_i\partial_{x_j}^2\left(\frac{k^2}{\varepsilon}\right)\right)\mathrm{d}x.\end{aligned}$$

Gathering up yields

$$
\begin{aligned}
&\int_\Omega \mathbf{v}\cdot\left(\nabla\cdot\left(\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\left(\nabla\delta\overline{\mathbf{u}}+\nabla\delta\overline{\mathbf{u}}^\top\right)\right)\right)\mathrm{d}x\\
=&\int_\Omega\sum_{i=1}^d\sum_{j=1}^d \delta\overline{u}_j\left(c_\mu\partial_{x_ix_j}\left(\frac{k^2}{\varepsilon}\right)v_i+c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_i}v_i+c_\mu\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_ix_j}v_i\right)\\
&\qquad+\delta\overline{u}_i\left(c_\mu\partial^2_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i+c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i+c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial^2_{x_j}v_i\right)\\
&\qquad-\delta\overline{u}_j\left(c_\mu\partial_{x_i}v_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)+c_\mu v_i\partial_{x_ix_j}\left(\frac{k^2}{\varepsilon}\right)\right)-\delta\overline{u}_i\left(c_\mu\partial_{x_j}v_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)+c_\mu v_i\partial^2_{x_j}\left(\frac{k^2}{\varepsilon}\right)\right)\mathrm{d}x\\
&+\int_\Gamma\sum_{i=1}^d\sum_{j=1}^d\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)v_i\partial_{x_i}\delta\overline{u}_jn_j-\delta\overline{u}_j\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i\right)n_i\\
&\qquad+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)v_i\partial_{x_j}\delta\overline{u}_in_j-\delta\overline{u}_i\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)v_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i\right)n_j\\
&\qquad+c_\mu v_i\delta\overline{u}_j\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)n_i+c_\mu v_i\delta\overline{u}_i\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)n_j\mathrm{d}s\\
=&\int_\Omega\sum_{i=1}^d\sum_{j=1}^d\delta\overline{u}_j\left(c_\mu\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_ix_j}v_i\right)+\delta\overline{u}_i\left(c_\mu\partial_{x_j}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial^2_{x_j}v_i\right)\mathrm{d}x\\
&+\int_\Gamma\sum_{i=1}^d\sum_{j=1}^d\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)v_i\partial_{x_i}\delta\overline{u}_jn_j-\delta\overline{u}_j\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v_in_i+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)v_i\partial_{x_j}\delta\overline{u}_in_j-\delta\overline{u}_i\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\partial_{x_j}v\\
=&\int_\Omega\sum_{i=1}^d\sum_{j=1}^d\left(c_\mu\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\left(\partial_{x_i}v_j+\partial_{x_j}v_i\right)+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\left(\partial_{x_ix_j}v_i+\partial^2_{x_i}v_j\right)\right)\delta\overline{u}_j\mathrm{d}x\\
&+\int_\Gamma\sum_{i=1}^d\sum_{j=1}^d\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\left(v_i\left(\partial_{x_i}\delta\overline{u}_j+\partial_{x_j}\delta\overline{u}_i\right)n_j-\delta\overline{u}_i\left(\partial_{x_i}v_j+\partial_{x_j}v_i\right)n_j\right)\mathrm{d}s\\
=&\int_\Omega 2c_\mu\nabla\left(\frac{k^2}{\varepsilon}\right)^\top\varepsilon(\mathbf{v})\delta\overline{\mathbf{u}}+\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\left(\nabla(\nabla\cdot\mathbf{v})+\Delta\mathbf{v}\right)\cdot\delta\overline{\mathbf{u}}\mathrm{d}x+\int_\Gamma 2\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\mathbf{v}^\top\varepsilon(\delta\overline{\mathbf{u}})\mathbf{n}-2\mathbf{n}^\top\varepsilon(\mathbf{v})\delta\mathbf{u}\mathrm{d}s.
\end{aligned}
$$

Divergence term.

$$\int_\Omega q\nabla\cdot\delta\overline{\mathbf{u}}\mathrm{d}x=-\int_\Omega\delta\overline{\mathbf{u}}\cdot\nabla q\mathrm{d}x+\int_\Gamma q\delta\overline{\mathbf{u}}\cdot\mathbf{n}\mathrm{d}s,$$

Term.

$$
\begin{aligned}
&\int_\Omega 2c_\mu r\frac{k^2}{\varepsilon}\left(\nabla\overline{\mathbf{u}}+\nabla\overline{\mathbf{u}}^\top\right):\nabla\delta\overline{\mathbf{u}}\mathrm{d}x=\int_\Omega 2c_\mu\sum_{i=1}^d\sum_{j=1}^d r\frac{k^2}{\varepsilon}\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\partial_{x_i}\delta\overline{u}_j\mathrm{d}x\\
=&\int_\Gamma 2c_\mu\sum_{i=1}^d\sum_{j=1}^d r\frac{k^2}{\varepsilon}\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\delta\overline{u}_jn_i\mathrm{d}s\\
&-\int_\Omega 2c_\mu\sum_{i=1}^d\sum_{j=1}^d\delta\overline{u}_j\left(\partial_{x_i}r\frac{k^2}{\varepsilon}\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)+r\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)+r\frac{k^2}{\varepsilon}\left(\partial^2_{x_i}\overline{u}_j+\partial_{x_ix_j}\overline{u}_i\right)\right)\mathrm{d}x
\end{aligned}
$$

$$= \int_\Gamma 4c_\mu r\frac{k^2}{\varepsilon}\mathbf{n}^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}}\mathrm{d}s - \int_\Omega 2c_\mu\left(2\frac{k^2}{\varepsilon}\nabla r^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} + 2r\nabla\left(\frac{k^2}{\varepsilon}\right)^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} + r\frac{k^2}{\varepsilon}\left(\Delta\overline{\mathbf{u}}\cdot\delta\overline{\mathbf{u}} + \nabla(\nabla\cdot\overline{\mathbf{u}})\cdot\delta\overline{\mathbf{u}}\right)\right)\mathrm{d}x.$$

Term.

$$\int_\Omega 2c_1\eta k\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right) : \nabla\delta\overline{\mathbf{u}}\mathrm{d}x = \int_\Omega 2c_1\sum_{i=1}^d\sum_{j=1}^d \eta k\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)\partial_{x_i}\delta\overline{u}_j\mathrm{d}x$$

$$= \int_\Gamma 2c_1\sum_{i=1}^d\sum_{j=1}^d \eta k\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)\delta\overline{u}_j n_i\mathrm{d}s$$

$$- \int_\Omega 2c_1\sum_{i=1}^d\sum_{j=1}^d \delta\overline{u}_j\left(\partial_{x_i}\eta k\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) + \eta\partial_{x_i}k\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) + \eta k\left(\partial^2_{x_i}\overline{u}_j + \partial_{x_ix_j}\overline{u}_i\right)\right)\mathrm{d}x$$

$$= \int_\Gamma 4c_1\eta k\mathbf{n}^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}}\mathrm{d}s - \int_\Omega 2c_1\left(2k\nabla\eta^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} + \eta\nabla k^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} + \eta k\left(\Delta\overline{\mathbf{u}}\cdot\delta\overline{\mathbf{u}} + \nabla(\nabla\cdot\overline{\mathbf{u}})\cdot\delta\overline{\mathbf{u}}\right)\right)\mathrm{d}x.$$

Term produced by $\nabla\overline{p}$.

$$-\int_\Omega \mathbf{v}\cdot\nabla\delta\overline{p}\mathrm{d}x = -\int_\Gamma \delta\overline{p}\mathbf{v}\cdot\mathbf{n}\mathrm{d}s + \int_\Omega \delta\overline{p}\nabla\cdot\mathbf{v}\mathrm{d}x.$$

Term. Since

$$\mathbf{v}\cdot\left(\nabla\cdot\left(2c_\mu\frac{k\delta k}{\varepsilon}\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right)\right)\right) = \mathbf{v}\cdot\left(\nabla\cdot\left(2c_\mu\frac{k\delta k}{\varepsilon}\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)_{i,j=1}^d\right)\right)$$

$$= \mathbf{v}\cdot\left(2c_\mu\frac{k\delta k}{\varepsilon}\left(\sum_{j=1}^d \partial_{x_ix_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right)_{i=1}^d + \left(\sum_{j=1}^d\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)2c_\mu\partial_{x_j}\left(\frac{k\delta k}{\varepsilon}\right)\right)_{i=1}^d\right)$$

$$= \sum_{i=1}^d 2c_\mu\frac{k\delta k}{\varepsilon}v_i\sum_{j=1}^d\left(\partial_{x_ix_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right) + v_i\sum_{j=1}^d\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)2c_\mu\left(\partial_{x_j}\left(\frac{k}{\varepsilon}\right)\delta k + \frac{k}{\varepsilon}\partial_{x_j}\delta k\right)$$

$$= \sum_{i=1}^d\sum_{j=1}^d 2c_\mu\frac{k\delta k}{\varepsilon}v_i\left(\partial_{x_ix_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right) + 2c_\mu v_i\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)\left(\partial_{x_j}\left(\frac{k}{\varepsilon}\right)\delta k + \frac{k}{\varepsilon}\partial_{x_j}\delta k\right),$$

hence

$$\int_\Omega \mathbf{v}\cdot\left(\nabla\cdot\left(2c_\mu\frac{k\delta k}{\varepsilon}\left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right)\right)\right)\mathrm{d}x$$

$$= \int_\Omega\sum_{i=1}^d\sum_{j=1}^d 2c_\mu\frac{k\delta k}{\varepsilon}v_i\left(\partial_{x_ix_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right) + 2c_\mu v_i\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)\left(\partial_{x_j}\left(\frac{k}{\varepsilon}\right)\delta k + \frac{k}{\varepsilon}\partial_{x_j}\delta k\right)\mathrm{d}x.$$

We only integrate by part the last term:

$$\int_\Omega\sum_{i=1}^d\sum_{j=1}^d 2c_\mu v_i\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)\frac{k}{\varepsilon}\partial_{x_j}\delta k\mathrm{d}x$$

$$= \int_\Gamma\sum_{i=1}^d\sum_{j=1}^d 2c_\mu v_i\left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right)\frac{k\delta k}{\varepsilon}n_j\mathrm{d}s$$

$$- \int_\Omega \sum_{i=1}^d \sum_{j=1}^d 2c_\mu \delta k \left(\partial_{x_j} v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \frac{k}{\varepsilon} + v_i \left(\partial_{x_i x_j} \overline{u}_j + \partial^2_{x_j} \overline{u}_i \right) \frac{k}{\varepsilon} + v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \partial_{x_j} \left(\frac{k}{\varepsilon} \right) \right) \mathrm{d}x.$$

Then

$$\begin{aligned}
&\int_\Omega \mathbf{v} \cdot \left(\nabla \cdot \left(2c_\mu \frac{k\delta k}{\varepsilon} \left(\nabla \overline{\mathbf{u}} + \nabla \overline{\mathbf{u}}^\top \right) \right) \right) \mathrm{d}x \\
=& \int_\Omega \sum_{i=1}^d \sum_{j=1}^d 2c_\mu \frac{k\delta k}{\varepsilon} v_i \left(\partial_{x_i x_j} \overline{u}_j + \partial^2_{x_j} \overline{u}_i \right) + 2c_\mu v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \partial_{x_j} \left(\frac{k}{\varepsilon} \right) \delta k \\
&\qquad - 2c_\mu \delta k \left(\partial_{x_j} v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \frac{k}{\varepsilon} + v_i \left(\partial_{x_i x_j} \overline{u}_j + \partial^2_{x_j} \overline{u}_i \right) \frac{k}{\varepsilon} + v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \partial_{x_j} \left(\frac{k}{\varepsilon} \right) \right) \mathrm{d}x \\
&+ \int_\Gamma \sum_{i=1}^d \sum_{j=1}^d 2c_\mu v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \frac{k\delta k}{\varepsilon} n_j \mathrm{d}s \\
=& -\int_\Omega \sum_{i=1}^d \sum_{j=1}^d 2c_\mu \delta k \partial_{x_j} v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \frac{k}{\varepsilon} \mathrm{d}x + \int_\Gamma \sum_{i=1}^d \sum_{j=1}^d 2c_\mu v_i \left(\partial_{x_i} \overline{u}_j + \partial_{x_j} \overline{u}_i \right) \frac{k\delta k}{\varepsilon} n_j \mathrm{d}s \\
=& -\int_\Omega 4c_\mu \frac{k\delta k}{\varepsilon} \varepsilon(\overline{\mathbf{u}}) : \nabla \mathbf{v} \mathrm{d}x + \int_\Gamma 4c_\mu \frac{k\delta k}{\varepsilon} \mathbf{v}^\top \varepsilon(\overline{\mathbf{u}}) \mathbf{n} \mathrm{d}s.
\end{aligned}$$

Term containing $\nabla \delta k$.

$$-\int_\Omega \mathbf{v} \cdot \frac{2}{3} \nabla \delta k \mathrm{d}x = -\int_\Gamma \frac{2}{3} \delta k \mathbf{v} \cdot \mathbf{n} \mathrm{d}s + \int_\Omega \frac{2}{3} \delta k \nabla \cdot \mathbf{v} \mathrm{d}x.$$

Term containing δk_t.

$$-\int_0^T \int_\Omega r \delta k_t \mathrm{d}x\mathrm{d}t = -\int_\Omega r(T)\delta k(T) - r(0)\delta k(0) \mathrm{d}x + \int_0^T \int_\Omega r_t \delta k \mathrm{d}x\mathrm{d}t.$$

Term.

$$\begin{aligned}
-\int_\Omega r \left(\left(\overline{\mathbf{u}} \cdot \nabla \right) \delta k \right) \mathrm{d}x &= -\int_\Omega r \sum_{i=1}^d \overline{u}_i \partial_{x_i} \delta k \mathrm{d}x = -\int_\Gamma r \sum_{i=1}^d \overline{u}_i \delta k n_i \mathrm{d}s + \int_\Omega \sum_{i=1}^d \delta k \left(\partial_{x_i} r \overline{u}_i + r \partial_{x_i} \overline{u}_i \right) \mathrm{d}x \\
&= -\int_\Gamma r \delta k \overline{\mathbf{u}} \cdot \mathbf{n} \mathrm{d}s + \int_\Omega \delta k \left(\nabla r \cdot \overline{\mathbf{u}} + r \nabla \cdot \overline{\mathbf{u}} \right) \mathrm{d}x = -\int_\Gamma r \delta k \overline{\mathbf{u}} \cdot \mathbf{n} \mathrm{d}s + \int_\Omega \delta k \nabla r \cdot \overline{\mathbf{u}} \mathrm{d}x.
\end{aligned}$$

Term.

$$\begin{aligned}
\int_\Omega r \nabla \cdot \left(2c_\mu \frac{k\delta k}{\varepsilon} \nabla k \right) \mathrm{d}x &= \int_\Gamma 2c_\mu r \frac{k\delta k}{\varepsilon} \nabla k \cdot \mathbf{n} \mathrm{d}s - \int_\Omega \nabla r \cdot \left(2c_\mu \frac{k\delta k}{\varepsilon} \nabla k \right) \mathrm{d}x \\
&= \int_\Gamma 2c_\mu r \frac{k\delta k}{\varepsilon} \nabla k \cdot \mathbf{n} \mathrm{d}s - \int_\Omega 2c_\mu \frac{k\delta k}{\varepsilon} \nabla r \cdot \nabla k \mathrm{d}x.
\end{aligned}$$

Term.

$$\int_\Omega r \nabla \cdot \left(c_\mu \frac{k^2}{\varepsilon} \nabla \delta k \right) \mathrm{d}x = \int_\Gamma c_\mu r \frac{k^2}{\varepsilon} \nabla \delta k \cdot \mathbf{n} \mathrm{d}s - \int_\Omega c_\mu \frac{k^2}{\varepsilon} \nabla r \cdot \nabla \delta k \mathrm{d}x.$$

We integrate by parts the last term

$$\begin{aligned} -\int_\Omega c_\mu \frac{k^2}{\varepsilon}\nabla r\cdot\nabla\delta k \mathrm{d}x &= -\int_\Omega c_\mu \frac{k^2}{\varepsilon}\sum_{i=1}^d \partial_{x_i} r\partial_{x_i}\delta k\mathrm{d}x \\ &= -\int_\Gamma c_\mu \frac{k^2}{\varepsilon}\sum_{i=1}^d \partial_{x_i} r\delta k n_i \mathrm{d}s + \int_\Omega c_\mu \sum_{i=1}^d \delta k\left(\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_i} r + \frac{k^2}{\varepsilon}\partial^2_{x_i} r\right)\mathrm{d}x. \end{aligned}$$

Hence

$$\begin{aligned} \int_\Omega r\nabla\cdot\left(c_\mu\frac{k^2}{\varepsilon}\nabla\delta k\right)\mathrm{d}x &= \int_\Gamma r c_\mu \frac{k^2}{\varepsilon}\nabla\delta k\cdot\mathbf{n}\mathrm{d}s - \int_\Gamma c_\mu\frac{k^2}{\varepsilon}\delta k\nabla r\cdot\mathbf{n}\mathrm{d}s + \int_\Omega c_\mu\delta k\left(\nabla\left(\frac{k^2}{\varepsilon}\right)\cdot\nabla r + \frac{k^2}{\varepsilon}\Delta r\right)\mathrm{d}x \\ &= \int_\Gamma c_\mu r\frac{k^2}{\varepsilon}\nabla\delta k\cdot\mathbf{n} - c_\mu\frac{k^2\delta k}{\varepsilon}\nabla r\cdot\mathbf{n}\mathrm{d}s + \int_\Omega c_\mu\delta k\left(\nabla\left(\frac{k^2}{\varepsilon}\right)\cdot\nabla r + \frac{k^2}{\varepsilon}\Delta r\right)\mathrm{d}x. \end{aligned}$$

Term.

$$\int_\Omega \eta\nabla\cdot\left(2c_\varepsilon\frac{k\delta k}{\varepsilon}\nabla\varepsilon\right)\mathrm{d}x = \int_\Gamma 2c_\varepsilon\eta\frac{k\delta k}{\varepsilon}\nabla\varepsilon\cdot\mathbf{n}\mathrm{d}s - \int_\Omega 2c_\varepsilon\frac{k\delta k}{\varepsilon}\nabla\eta\cdot\nabla\varepsilon\mathrm{d}x.$$

Second-order term. Since

$$\begin{aligned} &\mathbf{v}\cdot\left(\nabla\cdot\left(c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\left(\nabla\overline{\mathbf{u}}+\nabla\overline{\mathbf{u}}^\top\right)\right)\right) = \mathbf{v}\cdot\left(\nabla\cdot\left(c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)_{i,j=1}^d\right)\right) \\ &= \mathbf{v}\cdot\left(c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\left(\sum_{j=1}^d \partial_{x_ix_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right)_{i=1}^d + \left(\sum_{j=1}^d\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)c_\mu\partial_{x_j}\left(\frac{k^2\delta\varepsilon}{\varepsilon^2}\right)\right)_{i=1}^d\right) \\ &= \sum_{i=1}^d c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}v_i\sum_{j=1}^d\left(\partial_{x_ix_j}\overline{u}_j+\partial^2_{x_j}\overline{u}_i\right) + v_i\sum_{j=1}^d c_\mu\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\left(\partial_{x_j}\left(\frac{k^2}{\varepsilon^2}\right)\delta\varepsilon + \frac{k^2}{\varepsilon^2}\partial_{x_j}\delta\varepsilon\right) \\ &= \sum_{i=1}^d\sum_{j=1}^d c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}v_i\left(\partial_{x_ix_j}\overline{u}_j+\partial^2_{x_j}\overline{u}_i\right) + c_\mu v_i\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\left(\partial_{x_j}\left(\frac{k^2}{\varepsilon^2}\right)\delta\varepsilon + \frac{k^2}{\varepsilon^2}\partial_{x_j}\delta\varepsilon\right), \end{aligned}$$

hence

$$\begin{aligned} &\int_\Omega \mathbf{v}\cdot\left(\nabla\cdot\left(c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\left(\nabla\overline{\mathbf{u}}+\nabla\overline{\mathbf{u}}^\top\right)\right)\right)\mathrm{d}x \\ &= \int_\Omega\sum_{i=1}^d\sum_{j=1}^d c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}v_i\left(\partial_{x_ix_j}\overline{u}_j+\partial^2_{x_j}\overline{u}_i\right) + c_\mu v_i\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\left(\partial_{x_j}\left(\frac{k^2}{\varepsilon^2}\right)\delta\varepsilon + \frac{k^2}{\varepsilon^2}\partial_{x_j}\delta\varepsilon\right)\mathrm{d}x. \end{aligned}$$

We only integrate by part the last term:

$$\begin{aligned} &\int_\Omega\sum_{i=1}^d\sum_{j=1}^d c_\mu v_i\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\frac{k^2}{\varepsilon^2}\partial_{x_j}\delta\varepsilon\mathrm{d}x \\ &= \int_\Gamma\sum_{i=1}^d\sum_{j=1}^d c_\mu v_i\left(\partial_{x_i}\overline{u}_j+\partial_{x_j}\overline{u}_i\right)\frac{k^2}{\varepsilon^2}\delta\varepsilon n_j\mathrm{d}s \end{aligned}$$

$$-\int_\Omega \sum_{i=1}^d \sum_{j=1}^d c_\mu \delta\varepsilon \left(\partial_{x_j} v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \frac{k^2}{\varepsilon^2} + v_i \left(\partial_{x_i x_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right) \frac{k^2}{\varepsilon^2} + v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \partial_{x_j}\left(\frac{k^2}{\varepsilon^2}\right)\right) \mathrm{d}x.$$

Plugging back, we obtain

$$\begin{aligned}
&-\int_\Omega \mathbf{v} \cdot \left(\nabla \cdot \left(c_\mu \frac{k^2 \delta\varepsilon}{\varepsilon^2} \left(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top \right)\right)\right) \mathrm{d}x \\
&= -\int_\Omega \sum_{i=1}^d \sum_{j=1}^d c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} v_i \left(\partial_{x_i x_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right) + c_\mu v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \partial_{x_j}\left(\frac{k^2}{\varepsilon^2}\right)\delta\varepsilon \\
&\qquad - c_\mu \delta\varepsilon \left(\partial_{x_j} v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \frac{k^2}{\varepsilon^2} + v_i \left(\partial_{x_i x_j}\overline{u}_j + \partial^2_{x_j}\overline{u}_i\right) \frac{k^2}{\varepsilon^2} + v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \partial_{x_j}\left(\frac{k^2}{\varepsilon^2}\right)\right) \mathrm{d}x \\
&\quad - \int_\Gamma \sum_{i=1}^d \sum_{j=1}^d c_\mu v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \frac{k^2\delta\varepsilon}{\varepsilon^2} n_j \mathrm{d}s \\
&= \int_\Omega \sum_{i=1}^d \sum_{j=1}^d c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} \partial_{x_j} v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) \mathrm{d}x - \int_\Gamma \sum_{i=1}^d \sum_{j=1}^d c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} v_i \left(\partial_{x_i}\overline{u}_j + \partial_{x_j}\overline{u}_i\right) n_j \mathrm{d}s \\
&= \int_\Omega 2c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} \varepsilon(\overline{\mathbf{u}}) : \nabla\mathbf{v} \mathrm{d}x - \int_\Gamma 2c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} \mathbf{v}^\top \varepsilon(\overline{\mathbf{u}})\mathbf{n}\mathrm{d}s.
\end{aligned}$$

Term.

$$-\int_\Omega r\nabla \cdot \left(c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} \nabla k \right) \mathrm{d}x = \int_\Gamma c_\mu r \frac{k^2\delta\varepsilon}{\varepsilon^2} \nabla k \cdot \mathbf{n}\mathrm{d}s - \int_\Omega c_\mu \frac{k^2\delta\varepsilon}{\varepsilon^2} \nabla r \cdot \nabla k \mathrm{d}x.$$

Term containing $\delta\varepsilon_t$.

$$-\int_0^T \int_\Omega \eta \delta\varepsilon_t \mathrm{d}x\mathrm{d}t = -\int_\Omega \eta(T)\delta\varepsilon(T) - \eta(0)\delta\varepsilon(0)\mathrm{d}x + \int_0^T \int_\Omega \eta_t \delta\varepsilon \mathrm{d}x\mathrm{d}t.$$

Term.

$$\begin{aligned}
-\int_\Omega \eta \left(\left(\overline{\mathbf{u}} \cdot \nabla\right) \delta\varepsilon\right) \mathrm{d}x &= -\int_\Omega \eta \sum_{i=1}^d \overline{u}_i \partial_{x_i}\delta\varepsilon \mathrm{d}x = -\int_\Gamma \eta \sum_{i=1}^d \overline{u}_i \delta\varepsilon n_i \mathrm{d}s + \int_\Omega \sum_{i=1}^d \delta\varepsilon \left(\partial_{x_i}\eta\overline{u}_i + \eta\partial_{x_i}\overline{u}_i\right) \mathrm{d}x \\
&= -\int_\Gamma \eta\delta\varepsilon\overline{\mathbf{u}} \cdot \mathbf{n}\mathrm{d}s + \int_\Omega \delta\varepsilon \left(\nabla\eta \cdot \overline{\mathbf{u}} + \eta\nabla \cdot \overline{\mathbf{u}}\right) \mathrm{d}x = -\int_\Gamma \eta\delta\varepsilon\overline{\mathbf{u}} \cdot \mathbf{n}\mathrm{d}s + \int_\Omega \delta\varepsilon\nabla\eta \cdot \overline{\mathbf{u}}\mathrm{d}x.
\end{aligned}$$

Term.

$$-\int_\Omega \eta\nabla \cdot \left(c_\varepsilon \frac{k^2\delta\varepsilon}{\varepsilon^2} \nabla\varepsilon \right) \mathrm{d}x = -\int_\Gamma c_\varepsilon \eta \frac{k^2\delta\varepsilon}{\varepsilon^2} \nabla\varepsilon \cdot \mathbf{n}\mathrm{d}s + \int_\Omega c_\varepsilon \frac{k^2\delta\varepsilon}{\varepsilon^2} \nabla\eta \cdot \nabla\varepsilon \mathrm{d}x.$$

Last term.

$$\int_\Omega \eta\nabla \cdot \left(c_\varepsilon \frac{k^2}{\varepsilon} \nabla\delta\varepsilon \right) \mathrm{d}x = \int_\Gamma \eta c_\varepsilon \frac{k^2}{\varepsilon} \nabla\delta\varepsilon \cdot \mathbf{n}\mathrm{d}s - \int_\Omega c_\varepsilon \frac{k^2}{\varepsilon} \nabla\eta \cdot \nabla\delta\varepsilon \mathrm{d}x.$$

We integrate by part the last term:

$$\begin{aligned}
-\int_\Omega c_\varepsilon \frac{k^2}{\varepsilon}\nabla\eta\cdot\nabla\delta\varepsilon \mathrm{d}x &= -\int_\Omega c_\varepsilon \frac{k^2}{\varepsilon}\sum_{i=1}^d \partial_{x_i}\eta\partial_{x_i}\delta\varepsilon\mathrm{d}x \\
&= -\int_\Gamma c_\varepsilon \frac{k^2}{\varepsilon}\sum_{i=1}^d \partial_{x_i}\eta\delta\varepsilon n_i \mathrm{d}s + \int_\Omega c_\varepsilon \sum_{i=1}^d \delta\varepsilon\left(\partial_{x_i}\left(\frac{k^2}{\varepsilon}\right)\partial_{x_i}\eta + \frac{k^2}{\varepsilon}\partial^2_{x_i}\eta\right)\mathrm{d}x \\
&= -\int_\Gamma c_\varepsilon \frac{k^2\delta\varepsilon}{\varepsilon}\nabla\eta\cdot\mathbf{n}\mathrm{d}s + \int_\Omega c_\varepsilon\delta\varepsilon\left(\nabla\left(\frac{k^2}{\varepsilon}\right)\cdot\nabla\eta + \frac{k^2}{\varepsilon}\Delta\eta\right)\mathrm{d}x.
\end{aligned}$$

Plugging back, we obtain

$$\int_\Omega \eta\nabla\cdot\left(c_\varepsilon\frac{k^2}{\varepsilon}\nabla\delta\varepsilon\right)\mathrm{d}x = \int_\Gamma c_\varepsilon\eta\frac{k^2}{\varepsilon}\nabla\delta\varepsilon\cdot\mathbf{n}\mathrm{d}s - \int_\Gamma c_\varepsilon\frac{k^2\delta\varepsilon}{\varepsilon}\nabla\eta\cdot\mathbf{n}\mathrm{d}s + \int_\Omega c_\varepsilon\delta\varepsilon\left(\nabla\left(\frac{k^2}{\varepsilon}\right)\cdot\nabla\eta + \frac{k^2}{\varepsilon}\Delta\eta\right)\mathrm{d}x.$$

Gathering all terms, we can reformulate (3.20.2) as

$$\begin{aligned}
&\int_0^T\int_\Omega [\partial_{\overline{\mathbf{u}}}J_\Omega + \mathbf{v}_t + \nabla\overline{\mathbf{u}}\mathbf{v} + (\overline{\mathbf{u}}\cdot\nabla)\mathbf{v} + 2c_\mu\varepsilon(\mathbf{v})\nabla\left(\frac{k^2}{\varepsilon}\right) + \left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)(\nabla(\nabla\cdot\mathbf{v}) + \Delta\mathbf{v}) - \nabla q - r\nabla k \\
&\qquad - 4c_\mu\frac{k^2}{\varepsilon}\varepsilon(\overline{\mathbf{u}})\nabla r - 4c_\mu r\varepsilon(\overline{\mathbf{u}})\nabla\left(\frac{k^2}{\varepsilon}\right) - 2c_\mu r\frac{k^2}{\varepsilon}\Delta\overline{\mathbf{u}} - 2c_\mu\nabla\left(\nabla\cdot\overline{\mathbf{u}}\right) - \eta\nabla\varepsilon - 4c_1 k\varepsilon(\overline{\mathbf{u}})\nabla\eta \\
&\qquad - 2c_1\eta\varepsilon(\overline{\mathbf{u}})\nabla k - 2c_1\eta k\left(\Delta\overline{\mathbf{u}} + \nabla\left(\nabla\cdot\overline{\mathbf{u}}\right)\right)]\cdot\delta\overline{\mathbf{u}}\mathrm{d}x\mathrm{d}t \\
&+ \int_0^T\int_\Omega \left(\partial_{\overline{p}}J_\Omega + \nabla\cdot\mathbf{v}\right)\delta\overline{p}\mathrm{d}x\mathrm{d}t \\
&+ \int_0^T\int_\Omega [-4c_\mu\frac{k}{\varepsilon}\varepsilon(\overline{\mathbf{u}}):\nabla\mathbf{v} + \frac{2}{3}\nabla\cdot\mathbf{v} + r_t + \nabla r\cdot\overline{\mathbf{u}} - 2c_\mu\frac{k}{\varepsilon}\nabla r\cdot\nabla k + c_\mu\nabla\left(\frac{k^2}{\varepsilon}\right)\cdot\nabla r + c_\mu\frac{k^2}{\varepsilon}\Delta r \\
&\qquad + c_\mu r\frac{k}{\varepsilon}\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 - 2c_\varepsilon\frac{k}{\varepsilon}\nabla\eta\cdot\nabla\varepsilon + \frac{c_1}{2}\eta\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 + c_2\eta\frac{\varepsilon^2}{k^2}]\delta k\mathrm{d}x\mathrm{d}t \\
&+ \int_0^T\int_\Omega [2c_\mu\frac{k^2}{\varepsilon^2}\varepsilon(\overline{\mathbf{u}}):\nabla\mathbf{v} - c_\mu\frac{k^2}{\varepsilon^2}\nabla r\cdot\nabla k - \frac{c_\mu}{2}r\frac{k^2}{\varepsilon^2}\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 - r + \eta_t + \nabla\eta\cdot\overline{\mathbf{u}} + c_\varepsilon\frac{k^2}{\varepsilon^2}\nabla\eta\cdot\nabla\varepsilon \\
&\qquad + c_\varepsilon\nabla\left(\frac{k^2}{\varepsilon}\right)\cdot\nabla\eta + c_\varepsilon\frac{k^2}{\varepsilon}\Delta\eta - 2c_2\eta\frac{\varepsilon}{k}]\delta\varepsilon\mathrm{d}x\mathrm{d}t \\
&+ \int_\Omega\left[-\mathbf{v}(T)\cdot\delta\overline{\mathbf{u}}(T) + \mathbf{v}(0)\cdot\delta\overline{\mathbf{u}}(0) - r(T)\delta k(T) + r(0)\delta k(0) - \eta(T)\delta\varepsilon(T) + \eta(0)\delta\varepsilon(0)\right]\mathrm{d}x \\
&+ \int_0^T\int_\Gamma [\partial_{\overline{\mathbf{u}}}J_\Gamma\cdot\delta\overline{\mathbf{u}} + \partial_{\overline{p}}J_\Gamma\delta\overline{p} + 2\left(\nu + c_\mu\frac{k^2}{\varepsilon}\right)\mathbf{v}^\top\varepsilon(\delta\overline{\mathbf{u}})\mathbf{n} - 2\mathbf{n}^\top\varepsilon(\mathbf{v})\delta\overline{\mathbf{u}} + q\delta\overline{\mathbf{u}}\cdot\mathbf{n} + 4c_\mu r\frac{k^2}{\varepsilon}\mathbf{n}^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} \\
&\qquad + 4c_1\eta k\mathbf{n}^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} - \delta\overline{p}\mathbf{v}\cdot\mathbf{n} + 4c_\mu\frac{k\delta k}{\varepsilon}\mathbf{v}^\top\varepsilon(\overline{\mathbf{u}})\mathbf{n} - \frac{2}{3}\delta k\mathbf{v}\cdot\mathbf{n} - r\delta k\overline{\mathbf{u}}\cdot\mathbf{n} + 2c_\mu r\frac{k\delta k}{\varepsilon}\nabla k\cdot\mathbf{n} \\
&\qquad + c_\mu r\frac{k^2}{\varepsilon}\nabla\delta k\cdot\mathbf{n} - c_\mu\frac{k^2\delta k}{\varepsilon}\nabla r\cdot\mathbf{n} + 2c_\varepsilon\eta\frac{k\delta k}{\varepsilon}\nabla\varepsilon\cdot\mathbf{n} - 2c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\mathbf{v}^\top\varepsilon(\overline{\mathbf{u}})\mathbf{n} + c_\mu r\frac{k^2\delta\varepsilon}{\varepsilon^2}\nabla k\cdot\mathbf{n} \\
&\qquad - \eta\delta\varepsilon\overline{\mathbf{u}}\cdot\mathbf{n} - c_\varepsilon\eta\frac{k^2\delta\varepsilon}{\varepsilon^2}\nabla\varepsilon\cdot\mathbf{n} + c_\varepsilon\eta\frac{k^2}{\varepsilon}\nabla\delta\varepsilon\cdot\mathbf{n} - c_\varepsilon\frac{k^2\delta\varepsilon}{\varepsilon}\nabla\eta\cdot\mathbf{n}]\mathrm{d}x\mathrm{d}t.
\end{aligned}$$

Since this holds for any $\delta\overline{\mathbf{u}}, \delta\overline{p}, \delta k$ and $\delta\varepsilon$ satisfying the primal NSEs, the integrals vanish individually. The vanishing of the integrals over the domain yields the adjoint k-ε:

$$\begin{cases} \mathbf{v}_t + \left(\nu + c_\mu \dfrac{k^2}{\varepsilon}\right)(\nabla(\nabla\cdot\mathbf{v}) + \Delta\mathbf{v}) + 2c_\mu\varepsilon(\mathbf{v})\nabla\left(\dfrac{k^2}{\varepsilon}\right) + \nabla\overline{\mathbf{u}}\mathbf{v} + (\overline{\mathbf{u}}\cdot\nabla)\mathbf{v} - \nabla q \\ \qquad = -\partial_{\overline{\mathbf{u}}}J_\Omega + r\nabla k + 4c_\mu\dfrac{k^2}{\varepsilon}\varepsilon(\overline{\mathbf{u}})\nabla r + 4c_\mu r\varepsilon(\overline{\mathbf{u}})\nabla\left(\dfrac{k^2}{\varepsilon}\right) + 2c_\mu r\dfrac{k^2}{\varepsilon}\Delta\overline{\mathbf{u}} + 2c_\mu\nabla\left(\nabla\cdot\overline{\mathbf{u}}\right) + \eta\nabla\varepsilon \\ \qquad\quad + 4c_1k\varepsilon(\overline{\mathbf{u}})\nabla\eta + 2c_1\eta\varepsilon(\overline{\mathbf{u}})\nabla k + 2c_1\eta k\left(\Delta\overline{\mathbf{u}} + \nabla\left(\nabla\cdot\overline{\mathbf{u}}\right)\right) \text{ in } \Omega, \\ \nabla\cdot\mathbf{v} = -\partial_{\overline{p}}J_\Omega \text{ in } \Omega, \\ r_t + c_\mu\dfrac{k^2}{\varepsilon}\Delta r + \nabla r\cdot\overline{\mathbf{u}} - 2c_\mu\dfrac{k}{\varepsilon}\nabla r\cdot\nabla k + c_\mu\nabla\left(\dfrac{k^2}{\varepsilon}\right)\cdot\nabla r \\ \qquad = 4c_\mu\dfrac{k}{\varepsilon}\varepsilon(\overline{\mathbf{u}}) : \nabla\mathbf{v} - \dfrac{2}{3}\nabla\cdot\mathbf{v} - c_\mu r\dfrac{k}{\varepsilon}\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 + 2c_\varepsilon\dfrac{k}{\varepsilon}\nabla\eta\cdot\nabla\varepsilon - \dfrac{c_1}{2}\eta\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 - c_2\eta\dfrac{\varepsilon^2}{k^2} \text{ in } \Omega, \\ \eta_t + c_\varepsilon\dfrac{k^2}{\varepsilon}\Delta\eta + \nabla\eta\cdot\overline{\mathbf{u}} + c_\varepsilon\dfrac{k^2}{\varepsilon^2}\nabla\eta\cdot\nabla\varepsilon + c_\varepsilon\nabla\left(\dfrac{k^2}{\varepsilon}\right)\cdot\nabla\eta \\ \qquad = -2c_\mu\dfrac{k^2}{\varepsilon^2}\varepsilon(\overline{\mathbf{u}}) : \nabla\mathbf{v} + c_\mu\dfrac{k^2}{\varepsilon^2}\nabla r\cdot\nabla k + \dfrac{c_\mu}{2}r\dfrac{k^2}{\varepsilon^2}\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 + r + 2c_2\eta\dfrac{\varepsilon}{k} \text{ in } \Omega. \end{cases} \tag{6.3.1}$$

Plugging explicit formulas of J_Ω yields

$$\begin{aligned} J_\Omega(\overline{\mathbf{u}}, p) &= \gamma k_\epsilon\left(p + \frac{1}{2}|\overline{\mathbf{u}}|^2\right)\overline{\mathbf{u}}\cdot\mathbf{n}, \\ \partial_{\overline{\mathbf{u}}}J_\Omega(\overline{\mathbf{u}}, p) &= \gamma k_\epsilon\left(\left(p + \frac{1}{2}|\overline{\mathbf{u}}|^2\right)\mathbf{n} + (\overline{\mathbf{u}}\cdot\mathbf{n})\overline{\mathbf{u}}\right), \\ \partial_p J_\Omega(\overline{\mathbf{u}}, p) &= \gamma k_\epsilon\overline{\mathbf{u}}\cdot\mathbf{n}. \end{aligned}$$

Then (3.20.21) becomes

$$\begin{cases} \mathbf{v}_t + \left(\nu + c_\mu \dfrac{k^2}{\varepsilon}\right)(\nabla(\nabla\cdot\mathbf{v}) + \Delta\mathbf{v}) + 2c_\mu\varepsilon(\mathbf{v})\nabla\left(\dfrac{k^2}{\varepsilon}\right) + \nabla\overline{\mathbf{u}}\mathbf{v} + (\overline{\mathbf{u}}\cdot\nabla)\mathbf{v} - \nabla q \\ \qquad = -\gamma k_\epsilon\left(\left(p + \dfrac{1}{2}|\overline{\mathbf{u}}|^2\right)\mathbf{n} + (\overline{\mathbf{u}}\cdot\mathbf{n})\overline{\mathbf{u}}\right) + r\nabla k + 4c_\mu\dfrac{k^2}{\varepsilon}\varepsilon(\overline{\mathbf{u}})\nabla r + 4c_\mu r\varepsilon(\overline{\mathbf{u}})\nabla\left(\dfrac{k^2}{\varepsilon}\right) \\ \qquad\quad + 2c_\mu r\dfrac{k^2}{\varepsilon}\Delta\overline{\mathbf{u}} + 2c_\mu\nabla\left(\nabla\cdot\overline{\mathbf{u}}\right) + \eta\nabla\varepsilon + 4c_1k\varepsilon(\overline{\mathbf{u}})\nabla\eta + 2c_1\eta\varepsilon(\overline{\mathbf{u}})\nabla k + 2c_1\eta k\left(\Delta\overline{\mathbf{u}} + \nabla\left(\nabla\cdot\overline{\mathbf{u}}\right)\right) \text{ in } \Omega, \\ \nabla\cdot\mathbf{v} = -\gamma k_\epsilon\overline{\mathbf{u}}\cdot\mathbf{n} \text{ in } \Omega, \\ r_t + c_\mu\dfrac{k^2}{\varepsilon}\Delta r + \nabla r\cdot\overline{\mathbf{u}} - 2c_\mu\dfrac{k}{\varepsilon}\nabla r\cdot\nabla k + c_\mu\nabla\left(\dfrac{k^2}{\varepsilon}\right)\cdot\nabla r \\ \qquad = 4c_\mu\dfrac{k}{\varepsilon}\varepsilon(\overline{\mathbf{u}}) : \nabla\mathbf{v} - \dfrac{2}{3}\nabla\cdot\mathbf{v} - c_\mu r\dfrac{k}{\varepsilon}\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 + 2c_\varepsilon\dfrac{k}{\varepsilon}\nabla\eta\cdot\nabla\varepsilon - \dfrac{c_1}{2}\eta\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 - c_2\eta\dfrac{\varepsilon^2}{k^2} \text{ in } \Omega, \\ \eta_t + c_\varepsilon\dfrac{k^2}{\varepsilon}\Delta\eta + \nabla\eta\cdot\overline{\mathbf{u}} + c_\varepsilon\dfrac{k^2}{\varepsilon^2}\nabla\eta\cdot\nabla\varepsilon + c_\varepsilon\nabla\left(\dfrac{k^2}{\varepsilon}\right)\cdot\nabla\eta \\ \qquad = -2c_\mu\dfrac{k^2}{\varepsilon^2}\varepsilon(\overline{\mathbf{u}}) : \nabla\mathbf{v} + c_\mu\dfrac{k^2}{\varepsilon^2}\nabla r\cdot\nabla k + \dfrac{c_\mu}{2}r\dfrac{k^2}{\varepsilon^2}\left|\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^\top\right|^2 + r + 2c_2\eta\dfrac{\varepsilon}{k} \text{ in } \Omega. \end{cases} \tag{6.3.2}$$

The remaining terms yields

$$\int_\Omega [-\mathbf{v}(T)\cdot\delta\overline{\mathbf{u}}(T)+\mathbf{v}(0)\cdot\delta\overline{\mathbf{u}}(0)-r(T)\delta k(T)+r(0)\delta k(0)-\eta(T)\delta\varepsilon(T)+\eta(0)\delta\varepsilon(0)]\,\mathrm{d}x+\text{ICs for } k\text{-}\epsilon=0, \tag{6.3.3}$$

Wait initial conditions for k-ε!

and

$$\int_0^T\int_\Gamma[\partial_{\overline{\mathbf{u}}}J_\Gamma\cdot\delta\overline{\mathbf{u}}+\partial_{\overline{p}}J_\Gamma\delta\overline{p}+2\left(\nu+c_\mu\frac{k^2}{\varepsilon}\right)\mathbf{v}^\top\varepsilon(\delta\overline{\mathbf{u}})\mathbf{n}-2\mathbf{n}^\top\varepsilon(\mathbf{v})\delta\overline{\mathbf{u}}+q\delta\overline{\mathbf{u}}\cdot\mathbf{n}+4c_\mu r\frac{k^2}{\varepsilon}\mathbf{n}^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}} \tag{6.3.4}$$

$$+4c_1\eta k\mathbf{n}^\top\varepsilon(\overline{\mathbf{u}})\delta\overline{\mathbf{u}}-\delta\overline{p}\mathbf{v}\cdot\mathbf{n}+4c_\mu\frac{k\delta k}{\varepsilon}\mathbf{v}^\top\varepsilon(\overline{\mathbf{u}})\mathbf{n}-\frac{2}{3}\delta k\mathbf{v}\cdot\mathbf{n}-r\delta k\overline{\mathbf{u}}\cdot\mathbf{n}+2c_\mu r\frac{k\delta k}{\varepsilon}\nabla k\cdot\mathbf{n}+c_\mu r\frac{k^2}{\varepsilon}\nabla\delta k\cdot\mathbf{n} \tag{6.3.5}$$

$$-c_\mu\frac{k^2\delta k}{\varepsilon}\nabla r\cdot\mathbf{n}+2c_\varepsilon\eta\frac{k\delta k}{\varepsilon}\nabla\varepsilon\cdot\mathbf{n}-2c_\mu\frac{k^2\delta\varepsilon}{\varepsilon^2}\mathbf{v}^\top\varepsilon(\overline{\mathbf{u}})\mathbf{n}+c_\mu r\frac{k^2\delta\varepsilon}{\varepsilon^2}\nabla k\cdot\mathbf{n}-\eta\delta\varepsilon\overline{\mathbf{u}}\cdot\mathbf{n}-c_\varepsilon\eta\frac{k^2\delta\varepsilon}{\varepsilon^2}\nabla\varepsilon\cdot\mathbf{n} \tag{6.3.6}$$

$$+c_\varepsilon\eta\frac{k^2}{\varepsilon}\nabla\delta\varepsilon\cdot\mathbf{n}-c_\varepsilon\frac{k^2\delta\varepsilon}{\varepsilon}\nabla\eta\cdot\mathbf{n}]\mathrm{d}s\mathrm{d}t+\text{BCs for } k\text{-}\varepsilon=0. \tag{6.3.7}$$

Wait boundary conditions for k-ε!

Appendix A

Tools in Mathematical Analysis*

A.1 Differentiability in Banach spaces

See Tröltzsch, 2010, Chap. 2, Sect. 2.6.

Definition A.1.1 (1st variation). *Let $(U, \|\cdot\|_U)$ and $(V, \|\cdot\|_V)$ be Banach spaces, and $\mathcal{U}$ be a nonempty open subset of U, $u \in \mathcal{U}$ and $h \in U$, and $F : \mathcal{U} \subset U \to V$ be given. If the limit*

$$\delta F(u, h) \coloneqq \lim_{t \downarrow 0} \frac{1}{t} \left(F(u + th) - F(u) \right)$$

exists in V, then it is called the directional derivative *of F at u in the direction h.*

If this limit exists for all $h \in U$, then the mapping $h \mapsto \delta F(u, h)$ is termed the 1st variation *of F at u.*

Appendix B

Numerical Methods

In this chapter, we discuss some well-established methods for ODEs and PDEs.

B.1 Approximation of a normed space

First of all, we recall general concepts of approximation of a normed space presented in Temam, 2000, Subsect. I.3.1.

A normed space W must be approximated by a family $(W_h)_{h\in\mathcal{H}}$, where $\mathcal{H}$ is called the *set of indices*, of normed spaces W_h in any computational methods.

Definition B.1.1 (Internal approximation). *An* internal approximation *of a normed vector space W is a set consisting of a family of triples $\{W_h, p_h, r_h\}$, $h \in \mathcal{H}$ where*

(i) W_h is a normed vector space;

(ii) p_h is a linear continuous operator from W_h into W;

(iii) r_h is a (perhaps nonlinear) operator from W into W_h.

Definition B.1.2 (External approximation). *An* external approximation *of a normed space W is a set consisting of*

(i) a normed space F and an isomorphism $\overline{\omega}$ of W into F.

(ii) a family of triples $\{W_h, p_h, r_h\}_{h\in\mathcal{H}}$, in which, for each h,

- *W_h is a normed space,*
- *p_h a linear continuous mapping of W_h into F,*
- *r_h a (perhaps nonlinear) mapping of W into W_h.*

The operators p_h and r_h are called *prolongation* and *restriction operators*, respectively. When the spaces W and F are Hilbert spaces, and when the spaces W_h are likewise Hilbert spaces, the approximation is said to be a *Hilbert approximation*.

Definition B.1.3 ((Discrete/truncation) error). *For given $h, \mathbf{u} \in W$, $\mathbf{u}_h \in W_h$, we say that*

(i) $\|\overline{\omega}\mathbf{u} - p_h\mathbf{u}_h\|_F$ is the error *between $\mathbf{u}$ and $\mathbf{u}_h$,*

(ii) $\|\mathbf{u}_h - r_h\mathbf{u}\|_{W_h}$ is the discrete error *between $\mathbf{u}$ and $\mathbf{u}_h$,*

(iii) $\|\overline{\omega}\mathbf{u} - p_h r_h \mathbf{u}\|_F$ *is the* truncation error *of* $\mathbf{u}$.

We now define *stable* and *convergent approximations*.

Definition B.1.4 (Stable/convergent approximation)**.** *The prolongation operators p_h are said to be* stable *if their norms*

$$\|p_h\| = \sup_{u_h \in W_h,\, \|u_h\|_{W_h}=1} \|p_h \mathbf{u}_h\|_F$$

can be majorized independently of h.

The approximation of the space W is said to be stable *if the prolongation operators are stable.*

Definition B.1.5. *We will say that a family $\mathbf{u}_h$* converges strongly *(or* weakly*) to $\mathbf{u}$ if $p_h\mathbf{u}_h$ converges to $\overline{\omega}\mathbf{u}$ when $h \to 0$ in the strong (or weak) topology of F.*

We will say that the family $\mathbf{u}_h$ converges discretely *to $\mathbf{u}$ if*

$$\lim_{h\to 0} \|\mathbf{u}_h - r_h\mathbf{u}\|_{W_h} = 0.$$

Definition B.1.6. *We will say that an external approximation of a normed space W is* convergent *if the 2 following conditions hold:*

(C1) for all $\mathbf{u} \in W$

$$\lim_{h\to 0} p_h r_h \mathbf{u} = \overline{\omega}\mathbf{u}$$

in the strong topology of F.

(C2) for each sequence $\mathbf{u}'_h$ of elements of $W_{h'}$ ($h' \to 0$), s.t. $p_{h'}\mathbf{u}_{h'}$ converges to some element ϕ in the weak topology of F, we have, $\phi \in \overline{\omega}W$; i.e., $\phi = \overline{\omega}\mathbf{u}$ for some $\mathbf{u} \in W$.

Remark B.1.1. *Condition (C2) disappears when $\overline{\omega}$ is surjective and especially in the case of internal approximation.*

The following proposition shows that condition (C1) can in some sense be weakened for internal and external approximations.

Proposition B.1.1. *Let there be given a stable external approximation of a space W which is convergent in the following restrictive sense: the operators r_h are defined only on a dense subset $\mathcal{W}$ of W and condition (C1) in Definition 3.6 holds only for the $\mathbf{u}$ belonging to $\mathcal{W}$ (condition (C2) remains unchanged).*

Then it is possible to extend the definition of the restriction operators r_h to the whole space W so that condition (C1) is valid for each $\mathbf{u} \in W$ and hence the approximation of W is stable and convergent without any restriction.

Proof. See Temam, 2000, p. 30. □

Remark B.1.2. *If the mappings r_h are defined on the whole space W and condition (C1) holds for all $\mathbf{u} \in \mathcal{W}$, Proposition 3.1 shows us that we can modify the value of $r_h\mathbf{u}$ on the complement of $\mathcal{W}$ so that condition (C1) is satisfied for all $\mathbf{u} \in W$.*

B.1.1 A general convergence theorem

Let H be a Hilbert space, $a : H \times H \to \mathbb{R}$ be a coercive bilinear continuous form, and $\phi \in H^\star$. By Theorem 1.1.2, let $u \in H$ denote the unique solution of (1.1.1).

Let $\{H_h, p_h, r_h\}_{h\in\mathcal{H}}$ be an external stable and convergent Hilbert approximation of H. For each $h \in \mathcal{H}$, let there be given

(i) a continuous coercive bilinear form $a_h : H_h \times H_h \to \mathbb{R}$ and satisfies

$$\exists\alpha_0 > 0 \text{ independent of } h, \text{ s.t. } a_h(\mathbf{u}_h, \mathbf{u}_h) \geq \alpha_0\|\mathbf{u}_h\|^2_{H_h}, \ \forall\mathbf{u}_h \in H_h. \tag{B.1.1}$$

(ii) a continuous linear form $\phi_h \in H_h^\star$ such that

$$\|\phi_h\|_{H_h^\star} \leq \beta, \ \beta \text{ is independent of } h. \tag{B.1.2}$$

Now (1.1.1) is associated with the the following family of approximation equations:

For each $h \in \mathcal{H}$, find $u_h \in H_h$ such that

$$a_h(u_h, v_h) = \langle\phi_h, v_h\rangle, \ \forall v_h \in H_h. \tag{B.1.3}$$

By the preceding hypotheses, applying Theorem 1.1.2 for $(a, \phi, H) = (a_h, \phi_h, H_h)$ yields that (B.1.3) has a unique solution u_h, and we will call u_h an *approximate solution* of (1.1.1).

Assumption B.1.1 (Roger Temam's consistency hypotheses)**.** *(i) If $v_h \rightharpoonup v$ as $h \to 0$, and if $w_h \to w$ as $h \to 0$, then*

$$\lim_{h\to 0} a_h(v_h, w_h) = a(v, w), \ \lim_{h\to 0} a_h(w_h, v_h) = a(w, v). \tag{B.1.4}$$

(ii) If $v_h \rightharpoonup v$ as $h \to 0$, then

$$\lim_{h\to 0}\langle\phi_h, v_h\rangle = \langle\phi, v\rangle. \tag{B.1.5}$$

This is a manner in which the forms a_h and ϕ_h are consistent with the forms a and l. A general convergence theorem is stated as follows.

Theorem B.1.1. *Let H be a Hilbert space, $a(u, v)$ is a coercive bilinear continuous form on $H \times H$, $\phi \in H^\star$. Under the hypotheses (B.1.1), (B.1.2), (B.1.4), (B.1.5), the solution u_h of (B.1.3) converges strongly to the solution u of (1.1.1) as $h \to 0$.*

Proof. See Temam, 2000, pp. 32–33. □

Remark B.1.3. *For any $h \in \mathcal{H}$, if $\{w_{ih}\}_{1\leq i\leq N(h)}$ constitutes a basis of H_h, then the approximate problem (B.1.3) is equivalent to a regular linear system for the components of u_h in this basis; i.e., if $u_h \in H_h$ has the following representation*

$$u_h = \sum_{i=1}^{N(h)} \xi_{ih} w_{ih},$$

then (B.1.3) is equivalent to solving the following linear system

$$\sum_{i=1}^{N(h)} \xi_{ih} a_h(w_{ih}, w_{jh}) = \langle\phi_h, w_{jh}\rangle, \ 1 \leq j \leq N(h).$$

B.2 Finite Difference Methods

See, e.g., LeVeque, 2007. We denote $\mathbf{h} = (h_i)_{i=1}^N$ the *vector-mesh*, where h_i is the mesh in the x_i-direction and $0 < h_i \le h_i^0$, for $i = 1, \dots, N$. In this case, $\mathcal{H} = \prod_{i=1}^N (0, h_i^0)$.

B.3 Finite Element Methods*

B.4 Finite Volume Methods*

B.4.1 Finite Volume Meshes

B.4.1.1 Structured meshes

If Ω is a rectangle ($N = 2$) or a parallelepiped ($N = 3$), then it can be meshed with rectangular or parallelepipedic control volumes. For a regular structured mesh, every interior cell/control volume in the domain has the same number of neighboring cells.

Definition B.4.1 (Box in $\mathbb{R}^N$)**.** *Let $\mathbf{a}, \mathbf{b} \in \mathbb{R}^N$ such that $a_i < b_i$ for all $i = 1, \dots, N$. We define the box associated with $\mathbf{a}, \mathbf{b}$ as the Cartesian product of the intervals formed component-wise, i.e.,*

$$\mathrm{Box}(\mathbf{a}, \mathbf{b}) \coloneqq \prod_{i=1}^N [a_i, b_i] = [a_1, b_1] \times \cdots \times [a_N, b_N].$$

Definition B.4.2 (Rectangular admissible finite volume meshes for boxes in $\mathbb{R}^N$)**.** *Let $\mathbf{a}, \mathbf{b} \in \mathbb{R}^N$ such that $a_i < b_i$ for all $i = 1, \dots, N$. Let $(n_i)_{i=1}^N \in \mathbb{Z}_{>0}^N$. For each $i = 1, \dots, N$, let $h_{i,j} > 0$, $j = 1, \dots, n_i$ such that*

$$\sum_{j=1}^{n_i} h_{i,j} = b_i - a_i,$$

and let $h_{i,0} \coloneqq 0$, $h_{i,n_i+1} \coloneqq 0$, $x_{i,\frac{1}{2}} \coloneqq a_i$, $x_{i,j+\frac{1}{2}} \coloneqq x_{i,j-\frac{1}{2}} + h_{i,j}$ (so that $x_{i,n_i+\frac{1}{2}} = b_i$), and

$$\mathcal{T} \coloneqq (K_{j_1,\dots,j_N})_{j_1,\dots,j_N}^{n_1,\dots,n_N}, \ \text{where } K_{j_1,\dots,j_N} \coloneqq \prod_{i=1}^N [x_{i,j_i-\frac{1}{2}}, x_{i,j_i+\frac{1}{2}}];$$

let $(x_{i,j})_{j=0}^{n_i+1}$ such that $x_{i,j-\frac{1}{2}} < x_{i,j} < x_{i,j+\frac{1}{2}}$ for $j = 1, \dots, n_i$, $x_{i,0} \coloneqq a_i$, $x_{i,n_i+1} \coloneqq b_i$, and let $x_{j_1,\dots,j_N} \coloneqq (x_{1,j_1}, \dots, x_{N,j_N})$ for $j_1 = 1, \dots, n_i$; set

$$\begin{aligned} h_{i,j}^- \coloneqq x_{i,j} - x_{i,j-\frac{1}{2}}, \ h_{i,j}^+ \coloneqq x_{i,j+\frac{1}{2}} - x_j, &\quad \text{for } j = 1, \dots, n_i, \\ h_{i,j+\frac{1}{2}} \coloneqq x_{i,j+1} - x_{i,j}, &\quad \text{for } j = 0, \dots, n_i. \end{aligned}$$

Set $h \coloneqq \max\{h_{i,j}; i = 1, \dots, N; j = 1, \dots, n_i\}$.

Let $\mathcal{E}$ and $\mathcal{P}$ be the corresponding sets of edges and vertices of these rectangles. Then the triple $(\mathcal{T}, \mathcal{E}, \mathcal{P})$ is called a rectangular admissible finite volume meshes for $\mathrm{Box}(\mathbf{a}, \mathbf{b})$.

A particular case in 2D of the above definition is given in Eymard, Gallouët, and Herbin, 2019.

Definition B.4.3 (Rectangular admissible meshes in $\mathbb{R}^2$)**.** *Let $N_1 \in \mathbb{N}^\star$, $N_2 \in \mathbb{N}^\star$, $h_1, \dots, h_{N_1} > 0$, $k_1, \dots, k_{N_2} > 0$ s.t.*

$$\sum_{i=1}^{N_1} h_i = 1, \ \sum_{i=1}^{N_2} k_i = 1,$$

and let $h_0 = 0$, $h_{N_1+1} = 0$, $k_0 = 0$, $k_{N_2+1} = 0$.

For $i = 1, \dots, N_1$ let $x_{\frac{1}{2}} = 0$, $x_{i+\frac{1}{2}} = x_{i-\frac{1}{2}} + h_i$, (so that $x_{N_1+\frac{1}{2}} = 1$), and for $j = 1, \dots, N_2$, $y_{\frac{1}{2}} = 0$, $y_{j+\frac{1}{2}} = y_{i-\frac{1}{2}} + k_j$, (so that $y_{N_2+\frac{1}{2}} = 1$) and

$$K_{i,j} = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}].$$

Let $(x_i)_{i=0}^{N_1+1}$, and $(y_j)_{j=0}^{N_2+1}$, s.t.

$$x_{i-\frac{1}{2}} < x_i < x_{i+\frac{1}{2}}, \text{ for } i = 1, \dots, N_1, \ x_0 = 0, \ x_{N_1+1} = 1,$$
$$y_{j-\frac{1}{2}} < y_j < y_{j+\frac{1}{2}}, \text{ for } j = 1, \dots, N_2, \ y_0 = 0, \ y_{N_2+1} = 1,$$

and let $x_{i,j} = (x_i, y_j)$, for $i = 1, \dots, N_1$, $j = 1, \dots, N_2$; set

$$h_i^- = x_i - x_{i-\frac{1}{2}}, \ h_i^+ = x_{i+\frac{1}{2}} - x_i, \text{ for } i = 1, \dots, N_1, \ h_{i+\frac{1}{2}} = x_{i+1} - x_i, \text{ for } i = 0, \dots, N_1,$$
$$k_j^- = y_j - y_{j-\frac{1}{2}}, \ k_j^+ = y_{j+\frac{1}{2}} - y_j, \text{ for } j = 1, \dots, N_2, \ k_{j+\frac{1}{2}} = y_{j+1} - y_j, \text{ for } j = 0, \dots, N_2.$$

Let $h = \max\{(h_i, \ i = 1, \dots, N_1), (k_j, \ j = 1, \dots, N_2)\}$.

B.4.1.2 Unstructured meshes

We recall the following definition from Eymard, Gallouët, and Herbin, 2019, Definition 9.1, p. 37.

Definition B.4.4 (Admissible finite volume meshes)**.** *Let Ω be an open bounded polygonal subset of $\mathbb{R}^N$, $N \in \{2, 3\}$. An* admissible finite volume mesh *of Ω is defined as a triple $(\mathcal{T}, \mathcal{E}, \mathcal{P})$, where $\mathcal{T}$ is a family of "control volumes", which are open polygonal convex subsets of Ω, $\mathcal{E}$ is a family of subsets of $\overline{\Omega}$ contained in hyperplanes of $\mathbb{R}^N$ (these are the edges (2D) or sides (3D) of the control volumes) with strictly positive $(N-1)$-dimensional measure, and $\mathcal{P}$ is a family of points of Ω satisfying the following properties:*

(i) The closure of the union of all the control volumes is $\overline{\Omega}$;

(ii) For any $K \in \mathcal{T}$, there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ s.t. $\partial K = \overline{K} \backslash K = \bigcup_{\sigma \in \mathcal{E}_K} \overline{\sigma}$. Furthermore, $\mathcal{E} = \bigcup_{K \in \mathcal{T}} \mathcal{E}_K$.

(iii) For any $(K, L) \in \mathcal{T}^2$ with $K \neq L$, either the $(N-1)$-dimensional Lebesgue measure of $\overline{K} \cap \overline{L}$ is 0 or $\overline{K} \cap \overline{L} = \overline{\sigma}$ for some $\sigma \in \mathcal{E}$, which will then be denoted by $K|L$.

(iv) The family $\mathcal{P} = (\mathbf{x}_K)_{K \in \mathcal{T}}$ is s.t. $\mathbf{x}_K \in \overline{K}$ (for all $K \in \mathcal{T}$) and, if $\sigma = K|L$, it is assumed that $\mathbf{x}_K \neq \mathbf{x}_L$, and that the straight line $\mathcal{D}_{K,L}$ going through $\mathbf{x}_K$ and $\mathbf{x}_L$ is orthogonal to $K|L$.

(v) For any $\sigma \in \mathcal{E}$ s.t. $\sigma \subset \partial\Omega$, let K be the control volume s.t. $\sigma \in \mathcal{E}_K$. If $\mathbf{x}_K \notin \sigma$, let $\mathcal{D}_{K,\sigma}$ be the straight line going through $\mathbf{x}_K$ and orthogonal to σ, then the condition $\mathcal{D}_{K,\sigma} \cap \sigma \neq 0$ is assumed; let $\mathbf{y}_\sigma = \mathcal{D}_{K,\sigma} \cap \sigma$.

In the sequel, the following notations are used.

- The mesh size is defined by: $\mathrm{size}(\mathcal{T}) \coloneqq \sup\{\mathrm{diam}(K),\ K \in \mathcal{T}\}$.
- For any $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}$, $\mathrm{m}(K)$ is the N-dimensional Lebesgue measure of K (it is the area of K in the 2D case and the volume in the 3D case) and $\mathrm{H}_{N-1}(\sigma)$ the $(N-1)$-dimensional Hausdorff measure of σ.
- The set of interior (resp. boundary) edges is denoted by $\mathcal{E}_{\text{int}}$ (resp., $\mathcal{E}_{\text{ext}}$), i.e. $\mathcal{E}_{\text{int}} = \{\sigma \in \mathcal{E}; \sigma \not\subset \partial\Omega\}$ (resp., $\mathcal{E}_{\text{ext}} = \{\sigma \in \mathcal{E}; \sigma \subset \partial\Omega\}$).
- The set of neighbors of K is denoted by $\mathcal{N}(K)$, i.e. $\mathcal{N}(K) = \{L \in \mathcal{T}; \exists \sigma \in \mathcal{E}_K,\ \overline{\sigma} = \overline{K} \cap \overline{L}\}$.
- If $\sigma = K|L$, we denote d_σ or $d_{K|L}$ the Euclidean distance between $\mathbf{x}_K$ and $\mathbf{x}_L$ (which is positive) and by $d_{K,\sigma}$ the distance from $\mathbf{x}_K$ to σ.
- If $\sigma \in \mathcal{E}_K \cap \mathcal{E}_{\text{ext}}$, let d_σ denote the Euclidean distance between x_K and $\mathbf{y}_\sigma$ (then, $d_\sigma = d_{K,\sigma}$).
- For any $\sigma \in \mathcal{E}$; the "transmissibility" through σ is defined by $\tau_\sigma \coloneqq \frac{\mathrm{H}_{N-1}(\sigma)}{d_\sigma}$ if $d_\sigma \neq 0$.
- In some results and proofs given below, there are summations over $\sigma \in \mathcal{E}_0$, with $\mathcal{E}_0 \coloneqq \{\sigma \in \mathcal{E}; d_\sigma \neq 0\}$.

  For simplicity, (in these results and proofs) $\mathcal{E} = \mathcal{E}_0$ is assumed.

In Maz'ya and Rossmann, 2009, p. 673:

Definition B.4.5 (Domain of polyhedral type)**.** *The bounded domain $\mathcal{G} \subset \mathbb{R}^3$ is said to be a* domain of polyhedral type *if*

(i) The boundary $\partial\mathcal{G}$ consist of smooth (of class C^∞) open 2D manifolds Γ_j (the faces of $\mathcal{G}$), $j = 1, \dots, N$, smooth curves M_k (the edges), $k = 1, \dots, m$, and vertices $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(d)}$.

(ii) For every $\xi \in M_k$ there exist a neighborhood U_ξ and a diffeomorphism (a C^∞ mapping) κ_ξ which maps $\mathcal{G} \cap \mathcal{U}_\xi$ onto $\mathcal{D}_\xi \cap B_1$, where $\mathcal{D}_\xi$ is a dihedron of the form

$$\left\{\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3; 0 < r < \infty,\ -\frac{\theta}{2} < \varphi < \frac{\theta}{2},\ x_3 \in \mathbb{R}\right\},$$

and B_1 is the unit ball.

(iii) For every vertex $\mathbf{x}^{(j)}$ there exists a neighborhood $\mathcal{U}_j$ and a diffeomorphism κ_j mapping $\mathcal{G} \cap \mathcal{U}_j$ onto $\mathcal{K}_j \cap B_1$, where $\mathcal{K}_j$ is a polyhedral cone with vertex at the origin.

The set $M_1 \cup \cdots \cup M_m \cup \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(d)}\}$ of the singular boundary points is denoted by $\mathcal{S}$.
There are 3 types of indexing: local-, global-, and discretization indexings.

B.5 Mesh Generations*

B.5.1 OpenFOAM `blockMesh` utility

An duct geometry is generated by an OpenFOAM utility called `blockMesh`.

Appendix C

Terms Integrated by Parts in the Derivations of Adjoint Systems

This appendix is devoted to present a comprehensive list of the terms which are integrated by parts in the derivation of the adjoint systems. We consider below two cases: stationary and instationary cases, since in the latter, there will be the additional time integration.

C.1 Integration by parts formulas

C.1.1 Divergence theorem

Theorem C.1.1 (Divergence/Gauss-Green). *Given a bounded smooth domain D in $\mathbb{R}^N$ and a Lipschitzian domain Ω in D, then*

$$\forall \boldsymbol{\phi} \in C^1\left(\overline{D}, \mathbb{R}^N\right), \int_\Omega \nabla \cdot \boldsymbol{\phi} \mathrm{d}x = \int_\Gamma \boldsymbol{\phi} \cdot \mathbf{n} \mathrm{d}\Gamma, \tag{div}$$

where $\mathbf{n}$ *denotes the outward unit normal field.*

Lemma C.1.1 (Integration by parts). *If Ω is a bounded C^1 open set in $\mathbb{R}^N$ with boundary $\Gamma \coloneqq \partial\Omega$ and $v \in C^1(\overline{\Omega})$, $f \in C^1(\overline{\Omega})$, then*

$$\int_\Omega \nabla f \cdot \mathbf{v} \mathrm{d}\mathbf{x} = -\int_\Omega f \nabla \cdot \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma f \mathbf{v} \cdot \mathbf{n} \mathrm{d}\Gamma. \tag{ibp}$$

Proof. Use integration by parts formula for each component:

$$\begin{aligned}
\int_\Omega \nabla f \cdot \mathbf{v} \mathrm{d}\mathbf{x} &= \int_\Omega \sum_{i=1}^N \partial_{x_i} f v_i \mathrm{d}\mathbf{x} = \sum_{i=1}^N \int_\Omega \partial_{x_i} f v_i \mathrm{d}\mathbf{x} = \sum_{i=1}^N - \int_\Omega f \partial_{x_i} v_i \mathrm{d}\mathbf{x} + \int_\Gamma f v_i n_i \mathrm{d}\Gamma \\
&= -\int_\Omega f \sum_{i=1}^N \partial_{x_i} v_i \mathrm{d}\mathbf{x} + \int_\Gamma f \sum_{i=1}^N v_i n_i \mathrm{d}\Gamma = -\int_\Omega f \nabla \cdot \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma f \mathbf{v} \cdot \mathbf{n} \mathrm{d}\Gamma.
\end{aligned}$$

□

C.1.2 Green's identities for scalar functions

Lemma C.1.2 (Green's identities for scalar functions)**.** *If Ω is a bounded C^1 open set in $\mathbb{R}^N$ with boundary $\Gamma \coloneqq \partial\Omega$ and $u, v \in C^2(\overline{\Omega})$, then*

$$\int_\Omega \Delta uv\mathrm{d}\mathbf{x} = -\int_\Omega \nabla u \cdot \nabla v\mathrm{d}\mathbf{x} + \int_\Gamma \partial_\mathbf{n} uv\mathrm{d}\Gamma, \tag{1st-Green}$$

$$\int_\Omega \Delta uv\mathrm{d}\mathbf{x} = \int_\Omega u\Delta v\mathrm{d}\mathbf{x} + \int_\Gamma \partial_\mathbf{n} uv - u\partial_\mathbf{n} v\mathrm{d}\Gamma. \tag{2nd-Green}$$

About notation, Δuv means $(\Delta u)v$, not $\Delta(uv)$; also, $\partial_\mathbf{n} uv$ means $(\partial_\mathbf{n} u)v$, not $\partial_\mathbf{n}(uv)$.

Note that Green's first identity (1st-Green) is a special case of the more general identity derived from the divergence theorem C.1.1 by substituting $\boldsymbol{\phi} = \phi\mathbf{f}$ into (1st-Green):

$$\int_\Omega (\phi\nabla\cdot\mathbf{f} + \nabla\phi\cdot\mathbf{f})\,\mathrm{d}\mathbf{x} = \int_\Gamma \phi\mathbf{f}\cdot\mathbf{n}\mathrm{d}\Gamma. \tag{C.1.1}$$

C.1.3 Green's identities for vector fields

Lemma C.1.3 (Green's identities for vector fields)**.** *If Ω is a bounded C^1 open set in $\mathbb{R}^N$ with boundary $\Gamma \coloneqq \partial\Omega$ and $\mathbf{u}, \mathbf{v} \in C^2(\overline{\Omega}, \mathbb{R}^N)$, then*

$$\int_\Omega \Delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = -\int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\mathrm{d}\mathbf{x} + \int_\Gamma \partial_\mathbf{n}\mathbf{u}\cdot\mathbf{v}\mathrm{d}\Gamma, \tag{1st-Green-vec}$$

$$\int_\Omega \Delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{u}\cdot\Delta\mathbf{v}\mathrm{d}\mathbf{x} + \int_\Gamma (\partial_\mathbf{n}\mathbf{u}\cdot\mathbf{v} - \mathbf{u}\cdot\partial_\mathbf{n}\mathbf{v})\,\mathrm{d}\Gamma. \tag{2nd-Green-vec}$$

Proof. Use Green's identities for scalar functions to obtain the former:

$$\begin{aligned}\int_\Omega \Delta\mathbf{u}\cdot\mathbf{v}\mathrm{d}\mathbf{x} &= \int_\Omega \sum_{i=1}^N \Delta u_i v_i\mathrm{d}\mathbf{x} = \sum_{i=1}^N \int_\Omega \Delta u_i v_i\mathrm{d}\mathbf{x} = \sum_{i=1}^N -\int_\Omega \nabla u_i\cdot\nabla v_i\mathrm{d}\mathbf{x} + \int_\Gamma \partial_\mathbf{n} u_i v_i\mathrm{d}\Gamma \\ &= -\int_\Omega \sum_{i=1}^N \nabla u_i\cdot\nabla v_i\mathrm{d}\mathbf{x} + \int_\Gamma \sum_{i=1}^N \partial_\mathbf{n} u_i v_i\mathrm{d}\Gamma = -\int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\mathrm{d}\mathbf{x} + \int_\Gamma \partial_\mathbf{n}\mathbf{u}\cdot\mathbf{v}\mathrm{d}\Gamma.\end{aligned}$$

The latter is obtained by subtracting the former with its version after interchanging the roles of $\mathbf{u}$ and $\mathbf{v}$. □

C.1.4 Integration by parts involving matrices/2nd-order tensors

For a matrix/second-order tensor $A = (a_{ij})_{i,j=1}^{M,N} = (A_{i\cdot})_{i=1}^M = ((A_{\cdot j})_{j=1}^N)^\top \in C^1(\overline{\Omega}; \mathbb{R}^{M\times N})$ (where $A_{i\cdot}$ and $A_{\cdot j}$ is the ith row and jth column of A, respectively), its divergence is defined *column-wise*[1] by

$$\nabla\cdot A = (\nabla\cdot A_{\cdot j})_{j=1}^N = \left(\sum_{i=1}^M \partial_{x_i} a_{ij}\right)_{j=1}^N.$$

[1] In John, 2004 and John, 2016, the divergence of a matrix is defined *row-wise* instead.

Lemma C.1.4 (Integration by parts involving 2nd-order tensors)**.** *Let Ω be a bounded C^1 open set in $\mathbb{R}^N$ with boundary $\Gamma \coloneqq \partial\Omega$ and $A = (a_{ij})_{i,j=1}^N \in C^1(\overline{\Omega}, \mathbb{R}^{N^2})$, $\mathbf{v} \in C^1(\overline{\Omega}, \mathbb{R}^N)$, $f \in C^1(\overline{\Omega})$, then*

$$\int_\Omega (\nabla \cdot A) \cdot \mathbf{v} \mathrm{d}\mathbf{x} = -\int_\Omega A : \nabla \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top A \mathbf{v} \mathrm{d}\Gamma, \tag{ibp-mat1}$$

$$\int_\Omega \nabla \cdot (fA) \cdot \mathbf{v} \mathrm{d}\mathbf{x} = -\int_\Omega fA : \nabla \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma f\mathbf{n}^\top A \mathbf{v} \mathrm{d}\Gamma. \tag{ibp-mat2}$$

Moreover, if A is symmetric, then the following also holds:

$$\int_\Omega (\nabla \cdot A) \cdot \mathbf{v} \mathrm{d}\mathbf{x} = -\int_\Omega A : \boldsymbol{\varepsilon}(\mathbf{v}) \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top A \mathbf{v} \mathrm{d}\Gamma, \tag{ibp-mat3}$$

$$\int_\Omega \nabla \cdot (fA) \cdot \mathbf{v} \mathrm{d}\mathbf{x} = -\int_\Omega fA : \boldsymbol{\varepsilon}(\mathbf{v}) \mathrm{d}\mathbf{x} + \int_\Gamma f\mathbf{n}^\top A \mathbf{v} \mathrm{d}\Gamma, \tag{ibp-mat4}$$

Proof. Use integration by parts formula to obtain (ibp-mat1):

$$\begin{aligned}
\int_\Omega (\nabla \cdot A) \cdot \mathbf{v} \mathrm{d}\mathbf{x} &= \int_\Omega \left(\sum_{i=1}^N \partial_{x_i} a_{ij} \right)_{j=1}^N \cdot \mathbf{v} \mathrm{d}\mathbf{x} = \int_\Omega \sum_{j=1}^N \sum_{i=1}^N \partial_{x_i} a_{ij} v_j \mathrm{d}\mathbf{x} \\
&= \sum_{i=1}^N \sum_{j=1}^N \int_\Omega \partial_{x_i} a_{ij} v_j \mathrm{d}\mathbf{x} = \sum_{i=1}^N \sum_{j=1}^N - \int_\Omega a_{ij} \partial_{x_i} v_j \mathrm{d}\mathbf{x} + \int_\Gamma n_i a_{ij} v_j \mathrm{d}\Gamma \\
&= -\int_\Omega \sum_{i=1}^N \sum_{j=1}^N a_{ij} \partial_{x_i} v_j \mathrm{d}\mathbf{x} + \int_\Gamma \sum_{i=1}^N \sum_{j=1}^N n_i a_{ij} v_j \mathrm{d}\Gamma = -\int_\Omega A : \nabla \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top A \mathbf{v} \mathrm{d}\Gamma,
\end{aligned}$$

and (ibp-mat2) is obtained by applying the first one for $\widetilde{A} \coloneqq fA$.

If A is symmetric, i.e., $a_{ij} = a_{ji}$ for all $i, j = 1, \dots, N$, then

$$A : \nabla \mathbf{v} = \sum_{i=1}^N \sum_{j=1}^N a_{ij} \partial_{x_i} v_j = \sum_{i=1}^N \sum_{j=1}^N a_{ji} \partial_{x_j} v_i = \sum_{i=1}^N \sum_{j=1}^N a_{ij} \partial_{x_j} v_i,$$

and thus

$$A : \nabla \mathbf{v} = \sum_{i=1}^N \sum_{j=1}^N \frac{1}{2} a_{ij} (\partial_{x_i} v_j + \partial_{x_j} v_i) = \sum_{i=1}^N \sum_{j=1}^N a_{ij} \varepsilon_{ij}(\mathbf{v}) = A : \boldsymbol{\varepsilon}(\mathbf{v}).$$

Then (ibp-mat3) and (ibp-mat4) follow from (ibp-mat1) and (ibp-mat2), respectively. ☐

Corollary C.1.1 (Integration by parts involving 2nd-order tensors)**.** *Let Ω be a bounded C^1 open set in $\mathbb{R}^N$ with boundary $\Gamma \coloneqq \partial\Omega$ and $\mathbf{u} \in C^2(\overline{\Omega}, \mathbb{R}^N)$, $\mathbf{v} \in C^1(\overline{\Omega}, \mathbb{R}^N)$, $f \in C^1(\overline{\Omega})$, then*

$$\int_\Omega \nabla \cdot (f \nabla \mathbf{u}) \cdot \mathbf{v} \mathrm{d}\mathbf{x} = -\int_\Omega f \nabla \mathbf{u} : \nabla \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma f \partial_{\mathbf{n}} \mathbf{u} \cdot \mathbf{v} \mathrm{d}\Gamma, \tag{ibp-mat5}$$

$$\begin{aligned}
\int_\Omega \nabla \cdot (f \boldsymbol{\varepsilon}(\mathbf{u})) \cdot \mathbf{v} \mathrm{d}\mathbf{x} &= -\int_\Omega f \boldsymbol{\varepsilon}(\mathbf{u}) : \nabla \mathbf{v} \mathrm{d}\mathbf{x} + \int_\Gamma f \boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u}) \cdot \mathbf{v} \mathrm{d}\Gamma \\
&= -\int_\Omega f \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \mathrm{d}\mathbf{x} + \int_\Gamma f \boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u}) \cdot \mathbf{v} \mathrm{d}\Gamma.
\end{aligned} \tag{ibp-mat6}$$

If, in addition, $\mathbf{v} \in C^2(\overline{\Omega}, \mathbb{R}^N)$*, then*

$$\int_\Omega \nabla \cdot (f \nabla \mathbf{u}) \cdot \mathbf{v} d\mathbf{x} = \int_\Omega \nabla \cdot (f \nabla \mathbf{v}) \cdot \mathbf{u} d\mathbf{x} + \int_\Gamma f(\partial_\mathbf{n} \mathbf{u} \cdot \mathbf{v} - \mathbf{u} \cdot \partial_\mathbf{n} \mathbf{v}) d\Gamma, \tag{ibp-mat7}$$

$$\int_\Omega \nabla \cdot (f \boldsymbol{\varepsilon}(\mathbf{u})) \cdot \mathbf{v} d\mathbf{x} = \int_\Omega \nabla \cdot (f \boldsymbol{\varepsilon}(\mathbf{v})) \cdot \mathbf{u} d\mathbf{x} + \int_\Gamma f(\boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{u}) \cdot \mathbf{v} - \mathbf{u} \cdot \boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{v})) d\Gamma. \tag{ibp-mat8}$$

Proof. Applying (ibp-mat2) with $A = \nabla \mathbf{u}$ and $A = \boldsymbol{\varepsilon}(\mathbf{u})$ yields (ibp-mat5) and the first equality of (ibp-mat6), respectively. Applying (ibp-mat4) with $A = \boldsymbol{\varepsilon}(\mathbf{u})$ yields the second equality of (ibp-mat6).

Interchanging the role of $\mathbf{u}$ and $\mathbf{v}$ in (ibp-mat5) and the second equality of (ibp-mat6) yields

$$\int_\Omega \nabla \cdot (f \nabla \mathbf{v}) \cdot \mathbf{u} d\mathbf{x} = -\int_\Omega f \nabla \mathbf{u} : \nabla \mathbf{v} d\mathbf{x} + \int_\Gamma f \mathbf{u} \cdot \partial_\mathbf{n} \mathbf{v} d\Gamma,$$

$$\int_\Omega \nabla \cdot (f \boldsymbol{\varepsilon}(\mathbf{v})) \cdot \mathbf{u} d\mathbf{x} = -\int_\Omega f \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) d\mathbf{x} + \int_\Gamma f \mathbf{u} \cdot \boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{v}) d\Gamma.$$

Subtracting these with (ibp-mat5), (ibp-mat6) yields (ibp-mat7), (ibp-mat8), respectively. □

Remark C.1.1 (An integral identity)**.** *Interchanging the role of* $\mathbf{u}$ *and* $\mathbf{v}$ *in the first equality of* (ibp-mat6) *and then subtracting them yield also*

$$\int_\Omega \nabla \cdot (f \boldsymbol{\varepsilon}(\mathbf{u})) \cdot \mathbf{v} - \nabla \cdot (f \boldsymbol{\varepsilon}(\mathbf{v})) \cdot \mathbf{u} d\mathbf{x} = \int_\Omega f(\nabla \mathbf{u} : \boldsymbol{\varepsilon}(\mathbf{v}) - \boldsymbol{\varepsilon}(\mathbf{u}) : \nabla \mathbf{v}) d\mathbf{x} + \int_\Gamma f(\boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{u}) \cdot \mathbf{v} - \mathbf{u} \cdot \boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{v})) d\Gamma.$$

However, this identity is rarely used in this thesis.

C.2 Stationary Cases

1. **Diffusion term** $-\nabla \cdot (\nu \nabla \mathbf{u})$ **with** $\nu = \nu(\mathbf{x})$**.** Apply (ibp-mat5) with $f = \nu$ to obtain

$$-\int_\Omega \nabla \cdot (\nu \nabla \mathbf{u}) \cdot \mathbf{v} d\mathbf{x} = \int_\Omega \nu \nabla \mathbf{u} : \nabla \mathbf{v} d\mathbf{x} - \int_\Gamma \nu \partial_\mathbf{n} \mathbf{u} \cdot \mathbf{v} d\Gamma.$$

   Apply (ibp-mat7) with $f = \nu$ to obtain

$$-\int_\Omega \nabla \cdot (\nu \nabla \mathbf{u}) \cdot \mathbf{v} d\mathbf{x} = -\int_\Omega \nabla \cdot (\nu \nabla \mathbf{v}) \cdot \mathbf{u} d\mathbf{x} - \int_\Gamma \nu(\partial_\mathbf{n} \mathbf{u} \cdot \mathbf{v} - \mathbf{u} \cdot \partial_\mathbf{n} \mathbf{v}) d\Gamma.$$

2. **Diffusion term** $-\nu \Delta \mathbf{u}$**, with** $\nu =$ const**.** Integration by parts formulas for this term can be deduced directly from the previous term when by letting $\nu =$ const.

   Or, alternatively, we can apply (1st-Green-vec) to obtain

$$-\int_\Omega \nu \Delta \mathbf{u} \cdot \mathbf{v} d\mathbf{x} = \int_\Omega \nu \nabla \mathbf{u} : \nabla \mathbf{v} d\mathbf{x} - \int_\Gamma \nu \partial_\mathbf{n} \mathbf{u} \cdot \mathbf{v} d\Gamma.$$

   Apply (2nd-Green-vec) to obtain

$$-\int_\Omega \nu \Delta \mathbf{u} \cdot \mathbf{v} d\mathbf{x} = -\int_\Omega \nu \mathbf{u} \cdot \Delta \mathbf{v} d\mathbf{x} - \int_\Gamma \nu(\partial_\mathbf{n} \mathbf{u} \cdot \mathbf{v} - \mathbf{u} \cdot \partial_\mathbf{n} \mathbf{v}) d\Gamma.$$

3. **Diffusion term $-\nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{u}))$ with $\nu=\nu(\mathbf{x})$.** Apply (ibp-mat6) with $f=2\nu$ to obtain

$$-\int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{u}))\cdot\mathbf{v}\mathrm{d}\mathbf{x}=\int_\Omega 2\nu\boldsymbol{\varepsilon}(\mathbf{u}):\boldsymbol{\varepsilon}(\mathbf{v})\mathrm{d}\mathbf{x}-\int_\Gamma 2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u})\cdot\mathbf{v}\mathrm{d}\Gamma.$$

Apply (ibp-mat8) with $f=2\nu$ to obtain

$$-\int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{u}))\cdot\mathbf{v}\mathrm{d}\mathbf{x}=-\int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v}))\cdot\mathbf{u}\mathrm{d}\mathbf{x}-\int_\Gamma 2\nu(\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u})\cdot\mathbf{v}-\mathbf{u}\cdot\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{v}))\mathrm{d}\Gamma.$$

4. **Diffusion term $-2\nu\nabla\cdot\boldsymbol{\varepsilon}(\mathbf{u})$ with $\nu=\mathrm{const}$.** Integration by parts formulas for this term can be deduced directly from the previous term when by letting $\nu=\mathrm{const}$:

$$\begin{aligned}-\int_\Omega 2\nu\nabla\cdot\boldsymbol{\varepsilon}(\mathbf{u})\cdot\mathbf{v}\mathrm{d}\mathbf{x}&=\int_\Omega 2\nu\boldsymbol{\varepsilon}(\mathbf{u}):\boldsymbol{\varepsilon}(\mathbf{v})\mathrm{d}\mathbf{x}-\int_\Gamma 2\nu\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u})\cdot\mathbf{v}\mathrm{d}\Gamma,\\-\int_\Omega 2\nu\nabla\cdot\boldsymbol{\varepsilon}(\mathbf{u})\cdot\mathbf{v}\mathrm{d}\mathbf{x}&=-\int_\Omega 2\nu\nabla\cdot\boldsymbol{\varepsilon}(\mathbf{v})\cdot\mathbf{u}\mathrm{d}\mathbf{x}-\int_\Gamma 2\nu(\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{u})\cdot\mathbf{v}-\mathbf{u}\cdot\boldsymbol{\varepsilon}_{\mathbf{n}}(\mathbf{v}))\mathrm{d}\Gamma.\end{aligned}$$

5. **Convection term $(\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v}$.**

$$\begin{aligned}&\int_\Omega(\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v}\mathrm{d}\mathbf{x}=\int_\Omega\sum_{j=1}^N u_j\partial_{x_j}\mathbf{u}\cdot\mathbf{v}\mathrm{d}\mathbf{x}=\int_\Omega\sum_{j=1}^N\sum_{i=1}^N u_j\partial_{x_j}u_iv_i\mathrm{d}\mathbf{x}=\sum_{i=1}^N\sum_{j=1}^N\int_\Omega u_jv_i\partial_{x_j}u_i\mathrm{d}\mathbf{x}\\&=\sum_{i=1}^N\sum_{j=1}^N-\int_\Omega u_i\partial_{x_j}u_jv_i+u_iu_j\partial_{x_j}v_i\mathrm{d}\mathbf{x}+\int_\Gamma u_iv_iu_jn_j\mathrm{d}\Gamma\\&=-\int_\Omega\sum_{i=1}^N u_iv_i\sum_{j=1}^N\partial_{x_j}u_j+\sum_{i=1}^N\sum_{j=1}^N u_i\partial_{x_j}v_iu_j\mathrm{d}\mathbf{x}+\int_\Gamma\sum_{i=1}^N u_iv_i\sum_{j=1}^N u_jn_j\mathrm{d}\Gamma\\&=-\int_\Omega(\mathbf{u}\cdot\mathbf{v})\nabla\cdot\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{v}\cdot\mathbf{u}\mathrm{d}\mathbf{x}+\int_\Gamma(\mathbf{u}\cdot\mathbf{v})(\mathbf{u}\cdot\mathbf{n})\mathrm{d}\Gamma.\end{aligned}$$

6. **Convection term $\nabla\cdot(\mathbf{u}\otimes\mathbf{u})$.** Apply (ibp-mat1) with $A=\mathbf{u}\otimes\mathbf{u}$ to obtain

$$\int_\Omega\nabla\cdot(\mathbf{u}\otimes\mathbf{u})\cdot\mathbf{v}\mathrm{d}\mathbf{x}=-\int_\Omega(\mathbf{u}\otimes\mathbf{u}):\nabla\mathbf{v}\mathrm{d}\mathbf{x}+\int_\Gamma\mathbf{n}^\top(\mathbf{u}\otimes\mathbf{u})\mathbf{v}\mathrm{d}\Gamma.$$

7. **Gradient pressure term ∇p.** Apply (ibp) with $f=p$ to obtain

$$\int_\Omega\nabla p\cdot\mathbf{v}\mathrm{d}\mathbf{x}=-\int_\Omega p\nabla\cdot\mathbf{v}\mathrm{d}\mathbf{x}+\int_\Gamma p\mathbf{v}\cdot\mathbf{n}\mathrm{d}\Gamma.$$

8. **Domain cost term $D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}$.**

$$\begin{aligned}&\int_\Omega D_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}=\int_\Omega\nabla_{\nabla\mathbf{u}}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}\\&=\int_\Omega\sum_{i=1}^N\sum_{j=1}^N\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x}=\sum_{i=1}^N\sum_{j=1}^N\int_\Omega\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x}\\&=\sum_{i=1}^N\sum_{j=1}^N-\int_\Omega\partial_{x_i}\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\mathbf{x}+\int_\Gamma n_i\partial_{\partial_{x_i}u_j}J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\Gamma\end{aligned}$$

$$
\begin{aligned}
&= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \sum_{i=1}^N \partial_{x_i}\partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x} + \int_\Gamma \sum_{i=1}^N\sum_{j=1}^N n_i \partial_{\partial_{x_i}u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j \mathrm{d}\Gamma \\
&= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \nabla\cdot\left(\nabla_{\nabla u_j} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top \nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma \\
&= -\int_\Omega \nabla\cdot\left(\nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma \mathbf{n}^\top \nabla_{\nabla\mathbf{u}} J_\Omega(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma,
\end{aligned}
$$

where $\nabla_{\nabla\mathbf{u}} f(\nabla\mathbf{u}) \coloneqq \left(\partial_{\partial_{x_i}u_j} f(\nabla\mathbf{u})\right)_{i,j=1}^N$ for any scalar function $f:\mathbb{R}^{N^2}\to\mathbb{R}$.

9. **Diffusion term $D_\mathbf{u}(\mathrm{diff}(\nu,\mathbf{u}))\tilde{\mathbf{u}}\cdot\mathbf{v}$.** Apply (ibp-mat7) with $f=\nu$ and $\mathbf{u}=\tilde{\mathbf{u}}$ to obtain:

$$
\int_\Omega \nabla\cdot(\nu\nabla\tilde{\mathbf{u}})\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \nabla\cdot(\nu\nabla\mathbf{v})\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma \nu(\partial_\mathbf{n}\tilde{\mathbf{u}}\cdot\mathbf{v} - \tilde{\mathbf{u}}\cdot\partial_\mathbf{n}\mathbf{v})\mathrm{d}\Gamma.
$$

Apply (ibp-mat8) with $f=2\nu$ and $\mathbf{u}=\tilde{\mathbf{u}}$ to obtain:

$$
\int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\tilde{\mathbf{u}}))\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v}))\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma 2\nu(\boldsymbol{\varepsilon}_\mathbf{n}(\tilde{\mathbf{u}})\cdot\mathbf{v} - \tilde{\mathbf{u}}\cdot\boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{v}))\mathrm{d}\Gamma.
$$

Thus, $\int_\Omega D_\mathbf{u}(\mathrm{diff}(\nu,\mathbf{u}))\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\mathbf{x} =$

$$
= \begin{cases} \displaystyle\int_\Omega \nabla\cdot(\nu\nabla\mathbf{v})\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma \nu(\partial_\mathbf{n}\tilde{\mathbf{u}}\cdot\mathbf{v} - \tilde{\mathbf{u}}\cdot\partial_\mathbf{n}\mathbf{v})\mathrm{d}\Gamma, & \text{if } \mathrm{diff}(\nu,\mathbf{u}) = \nabla\cdot(\nu\nabla\mathbf{u}), \\ \displaystyle\int_\Omega \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{v}))\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} + \int_\Gamma 2\nu(\boldsymbol{\varepsilon}_\mathbf{n}(\tilde{\mathbf{u}})\cdot\mathbf{v} - \tilde{\mathbf{u}}\cdot\boldsymbol{\varepsilon}_\mathbf{n}(\mathbf{v}))\mathrm{d}\Gamma, & \text{if } \mathrm{diff}(\nu,\mathbf{u}) = \nabla\cdot(2\nu\boldsymbol{\varepsilon}(\mathbf{u})). \end{cases}
$$

10. **Domain cost term $D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}$.**

$$
\begin{aligned}
&\int_\Omega D_{\nabla\mathbf{u}}\mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \left(\nabla_{\nabla\mathbf{u}} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\tilde{\mathbf{u}}\right)_{k=1}^N\cdot\mathbf{v}\mathrm{d}\mathbf{x} \\
&= \int_\Omega \sum_{k=1}^N \nabla_{\nabla\mathbf{u}} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p):\nabla\tilde{\mathbf{u}} v_k\mathrm{d}\mathbf{x} = \int_\Omega \sum_{k=1}^N\sum_{i=1}^N\sum_{j=1}^N \partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j v_k\mathrm{d}\mathbf{x} \\
&= \sum_{i=1}^N\sum_{j=1}^N\sum_{k=1}^N \int_\Omega \partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j v_k\mathrm{d}\mathbf{x} \\
&= \sum_{i=1}^N\sum_{j=1}^N\sum_{k=1}^N - \int_\Omega \partial_{x_i}\partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j v_k + \partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\partial_{x_i} v_k\mathrm{d}\mathbf{x} \\
&\quad + \int_\Gamma n_i\partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j v_k\mathrm{d}\Gamma \\
&= -\int_\Omega \sum_{j=1}^N \tilde{u}_j\sum_{k=1}^N v_k\sum_{i=1}^N \partial_{x_i}\partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) + \sum_{j=1}^N\tilde{u}_j\sum_{k=1}^N\sum_{i=1}^N \partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i} v_k\mathrm{d}\mathbf{x} \\
&\quad + \int_\Gamma \sum_{j=1}^N\tilde{u}_j\sum_{k=1}^N v_k\sum_{i=1}^N n_i\partial_{\partial_{x_i}u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\Gamma
\end{aligned}
$$

$$= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N v_k \nabla \cdot \left(\nabla_{\nabla u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right) + \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N \nabla_{\nabla u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \cdot \nabla v_k \mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma \sum_{j=1}^N \tilde{u}_j \sum_{k=1}^N v_k \nabla_{\nabla u_j} f_k(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \cdot \mathbf{n} \mathrm{d}\Gamma$$
$$= -\int_\Omega \sum_{j=1}^N \tilde{u}_j \nabla \cdot \left(\nabla_{\nabla u_j} \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right) \cdot \mathbf{v} + \sum_{j=1}^N \tilde{u}_j \nabla_{\nabla u_j} \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v}\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma \sum_{j=1}^N \tilde{u}_j \left(\nabla_{\nabla u_j} \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \cdot \mathbf{n}\right) \cdot \mathbf{v}\mathrm{d}\Gamma$$
$$= -\int_\Omega \left(\nabla \cdot (\nabla_{\nabla\mathbf{u}} \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)) \cdot \mathbf{v}\right) \cdot \tilde{\mathbf{u}} + (\nabla_{\nabla\mathbf{u}} \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\mathbf{v}) \cdot \tilde{\mathbf{u}}\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma ((\nabla_{\nabla\mathbf{u}} \mathbf{f}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) \cdot \mathbf{n}) \cdot \mathbf{v}) \cdot \tilde{\mathbf{u}}\mathrm{d}\Gamma.$$

11. **Term $-\nabla\tilde{p}\cdot\mathbf{v}$.** Apply (ibp) with $f = \tilde{p}$ to obtain:

$$-\int_\Omega \nabla\tilde{p}\cdot\mathbf{v}\mathrm{d}\mathbf{x} = \int_\Omega \tilde{p}\nabla\cdot\mathbf{v}\mathrm{d}\mathbf{x} - \int_\Gamma \tilde{p}\mathbf{v}\cdot\mathbf{n}\mathrm{d}\Gamma.$$

12. **Term $-q\nabla\cdot\tilde{\mathbf{u}}$.** Apply (ibp) with $f = q$ and $\mathbf{v} = \tilde{\mathbf{u}}$ to obtain:

$$-\int_\Omega q\nabla\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = \int_\Omega \nabla q\cdot\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} - \int_\Gamma q\tilde{\mathbf{u}}\cdot\mathbf{n}\mathrm{d}\Gamma.$$

13. **Term $qD_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}$.**

$$\int_\Omega qD_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x} = \int_\Omega q\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p) : \nabla\tilde{\mathbf{u}}\mathrm{d}\mathbf{x}$$
$$= \int_\Omega q\sum_{i=1}^N\sum_{j=1}^N \partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x} = \sum_{i=1}^N\sum_{j=1}^N \int_\Omega q\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\partial_{x_i}\tilde{u}_j\mathrm{d}\mathbf{x}$$
$$= \sum_{i=1}^N\sum_{j=1}^N - \int_\Omega \partial_{x_i} q\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j + q\partial_{x_i}\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma qn_i\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\Gamma$$
$$= -\int_\Omega \sum_{i=1}^N\sum_{j=1}^N \partial_{x_i} q\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j + q\sum_{j=1}^N \tilde{u}_j \sum_{i=1}^N \partial_{x_i}\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma q\sum_{i=1}^N\sum_{j=1}^N n_i\partial_{\partial_{x_i}u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{u}_j\mathrm{d}\Gamma$$
$$= -\int_\Omega \nabla^\top q\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}} + q\sum_{j=1}^N \tilde{u}_j \nabla\cdot\left(\nabla_{\nabla u_j} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\right)\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma q\mathbf{n}^\top\nabla_{\nabla\mathbf{u}} f_{\mathrm{div}}(\mathbf{x},\mathbf{u},\nabla\mathbf{u},p)\tilde{\mathbf{u}}\mathrm{d}\Gamma$$

$$= -\int_\Omega \nabla^\top q \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)\tilde{\mathbf{u}} + q\left(\nabla \cdot \left(\nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)\right)\right) \cdot \tilde{\mathbf{u}} \mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma q \mathbf{n}^\top \nabla_{\nabla \mathbf{u}} f_{\mathrm{div}}(\mathbf{x}, \mathbf{u}, \nabla \mathbf{u}, p)\tilde{\mathbf{u}} \mathrm{d}\Gamma.$$

C.3 Instationary Cases

1. **Term $\partial_t \mathbf{u}$.**

$$\begin{aligned}
\int_0^T \int_\Omega \partial_t \mathbf{u} \cdot \mathbf{v} \mathrm{d}\mathbf{x}\mathrm{d}t &= \int_\Omega \int_0^T \sum_{i=1}^N \partial_t u_i v_i \mathrm{d}t\mathrm{d}\mathbf{x} = \int_\Omega \sum_{i=1}^N \int_0^T \partial_t u_i v_i \mathrm{d}t\mathrm{d}\mathbf{x} \\
&= \int_\Omega \left(\sum_{i=1}^N u_i(T)v_i(T) - u_i(0)v_i(0) - \int_0^T u_i \partial_t v_i \mathrm{d}t \right) \mathrm{d}\mathbf{x} \\
&= \int_\Omega \left(\mathbf{u}(T) \cdot \mathbf{v}(T) - \mathbf{u}(0) \cdot \mathbf{v}(0) - \int_0^T \sum_{i=1}^N u_i \partial_t v_i \mathrm{d}t \right) \mathrm{d}\mathbf{x} \\
&= \int_\Omega \mathbf{u}(T) \cdot \mathbf{v}(T) - \mathbf{u}_0 \cdot \mathbf{v}(0) \mathrm{d}\mathbf{x} - \int_0^T \int_\Omega \mathbf{u} \cdot \partial_t \mathbf{v} \mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}$$

2. **Term $\partial_t(\rho \mathbf{u})$.** Apply the previous one with $\mathbf{u}$ replaced by $\rho \mathbf{u}$ to obtain

$$\int_0^T \int_\Omega \partial_t(\rho \mathbf{u}) \cdot \mathbf{v} \mathrm{d}\mathbf{x}\mathrm{d}t = \int_\Omega \rho(T)\mathbf{u}(T) \cdot \mathbf{v}(T) - \rho(0)\mathbf{u}(0) \cdot \mathbf{v}(0) \mathrm{d}\mathbf{x} - \int_0^T \int_\Omega \rho \mathbf{u} \cdot \partial_t \mathbf{v} \mathrm{d}\mathbf{x}\mathrm{d}t.$$

3. **Convective term $\nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u})$.** Apply (ibp-mat1) with $A = \rho \mathbf{u} \otimes \mathbf{u}$ to obtain

$$\int_0^T \int_\Omega \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) \cdot \mathbf{v} \mathrm{d}\mathbf{x}\mathrm{d}t = -\int_0^T \int_\Omega \rho(\mathbf{u} \otimes \mathbf{u}) : \nabla \mathbf{v} \mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T \int_\Gamma \mathbf{n}^\top \rho(\mathbf{u} \otimes \mathbf{u})\mathbf{v} \mathrm{d}\Gamma\mathrm{d}t.$$

Bibliography

Alt, Hans Wilhelm (2016). *Linear functional analysis*. Universitext. An application-oriented introduction, Translated from the German edition by Robert Nürnberg. Springer-Verlag London, Ltd., London, pp. xii+435. ISBN: 978-1-4471-7279-6; 978-1-4471-7280-2. DOI: 10.1007/978-1-4471-7280-2. URL: https://doi.org/10.1007/978-1-4471-7280-2.

Brezis, Haim (2011). *Functional analysis, Sobolev spaces and partial differential equations*. Universitext. Springer, New York, pp. xiv+599. ISBN: 978-0-387-70913-0.

Céa, Jean (1986). "Conception optimale ou identification de formes: calcul rapide de la dérivée directionnelle de la fonction coût". In: *RAIRO Modél. Math. Anal. Numér.* 20.3, pp. 371–402. ISSN: 0764-583X. DOI: 10.1051/m2an/1986200303711. URL: https://doi.org/10.1051/m2an/1986200303711.

Chacón Rebollo, Tomás and Roger Lewandowski (2014). *Mathematical and numerical foundations of turbulence models and applications*. Modeling and Simulation in Science, Engineering and Technology. Birkhäuser/Springer, New York, pp. xviii+517. ISBN: 978-1-4939-0454-9; 978-1-4939-0455-6. DOI: 10.1007/978-1-4939-0455-6. URL: https://doi.org/10.1007/978-1-4939-0455-6.

Delfour, M. C. (2012). *Introduction to optimization and semidifferential calculus*. Vol. 12. MOS-SIAM Series on Optimization. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA; Mathematical Optimization Society, Philadelphia, PA, pp. xvi+353. ISBN: 978-1-611972-14-6. DOI: 10.1137/1.9781611972153. URL: https://doi.org/10.1137/1.9781611972153.

Delfour, M. C. and J.-P. Zolésio (1988a). "Shape sensitivity analysis via a penalization method". In: *Ann. Mat. Pura Appl. (4)* 151, pp. 179–212. ISSN: 0003-4622. DOI: 10.1007/BF01762794. URL: https://doi.org/10.1007/BF01762794.

— (1988b). "Shape sensitivity analysis via min max differentiability". In: *SIAM J. Control Optim.* 26.4, pp. 834–862. ISSN: 0363-0129. DOI: 10.1137/0326048. URL: https://doi.org/10.1137/0326048.

Eymard, Robert, Thierry Gallouët, and Raphaèle Herbin (2019). "Finite Volume Methods". In: *Handbook of Numerical Analysis, P.G. Ciarlet, J.L. Lions eds, 1997*. Vol. 7, pp. 713–1020. URL: https://hal.archives-ouvertes.fr/hal-02100732v2.

Ferziger, Joel H., Milovan Perić, and Robert L. Street (2020). *Computational methods for fluid dynamics*. Fourth edition. Springer, Cham, pp. xviii+596. ISBN: 978-3-319-99691-2; 978-3-319-99693-6. DOI: 10.1007/978-3-319-99693-6. URL: https://doi.org/10.1007/978-3-319-99693-6.

Gunzburger, Max D. (1989). *Finite element methods for viscous incompressible flows*. Computer Science and Scientific Computing. A guide to theory, practice, and algorithms. Academic Press, Inc., Boston, MA, pp. xviii+269. ISBN: 0-12-307350-2.

Hintermüller, Michael et al. (2004). "Dynamical systems-based optimal control of incompressible fluids". In: *Internat. J. Numer. Methods Fluids* 46.4, pp. 345–359. ISSN: 0271-2091. DOI: 10.1002/fld.725. URL: https://doi.org/10.1002/fld.725.

Isaacson, Eugene and Herbert Bishop Keller (1994). *Analysis of numerical methods.* Corrected reprint of the 1966 original [Wiley, New York; MR0201039 (34 #924)]. Dover Publications, Inc., New York, pp. xvi+541. ISBN: 0-486-68029-0.

Ito, Kazufumi, Karl Kunisch, and Gunther H. Peichl (2006). "Variational approach to shape derivatives for a class of Bernoulli problems". In: *J. Math. Anal. Appl.* 314.1, pp. 126–149. ISSN: 0022-247X. DOI: 10.1016/j.jmaa.2005.03.100. URL: https://doi.org/10.1016/j.jmaa.2005.03.100.

— (2008). "Variational approach to shape derivatives". In: *ESAIM Control Optim. Calc. Var.* 14.3, pp. 517–539. ISSN: 1292-8119. DOI: 10.1051/cocv:2008002. URL: https://doi.org/10.1051/cocv:2008002.

John, Volker (2004). *Large eddy simulation of turbulent incompressible flows.* Vol. 34. Lecture Notes in Computational Science and Engineering. Analytical and numerical results for a class of LES models. Springer-Verlag, Berlin, pp. xii+261. ISBN: 3-540-40643-3. DOI: 10.1007/978-3-642-18682-0. URL: https://doi.org/10.1007/978-3-642-18682-0.

— (2016). *Finite element methods for incompressible flow problems.* Vol. 51. Springer Series in Computational Mathematics. Springer, Cham, pp. xiii+812. ISBN: 978-3-319-45749-9; 978-3-319-45750-5. DOI: 10.1007/978-3-319-45750-5. URL: https://doi.org/10.1007/978-3-319-45750-5.

Kasumba, Henry (2010). "Optimal shape design using translation invariant cost functionals in fluid dynamics". PhD Thesis, Karl-Franzens University Graz. PhD thesis, pp. xiv+158.

LeVeque, Randall J. (2002). *Finite volume methods for hyperbolic problems.* Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge, pp. xx+558. ISBN: 0-521-81087-6; 0-521-00924-3. DOI: 10.1017/CBO9780511791253. URL: https://doi.org/10.1017/CBO9780511791253.

— (2007). *Finite difference methods for ordinary and partial differential equations.* Steady-state and time-dependent problems. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, pp. xvi+341. ISBN: 978-0-898716-29-0. DOI: 10.1137/1.9780898717839. URL: https://doi.org/10.1137/1.9780898717839.

Lions, J.-L. and E. Magenes (1972). *Non-homogeneous boundary value problems and applications. Vol. I.* Die Grundlehren der mathematischen Wissenschaften, Band 181. Translated from the French by P. Kenneth. Springer-Verlag, New York-Heidelberg, pp. xvi+357.

Maz'ya, V. and J. Rossmann (2005). "Pointwise estimates for Green's kernel of a mixed boundary value problem to the Stokes system in a polyhedral cone". In: *Math. Nachr.* 278.15, pp. 1766–1810. ISSN: 0025-584X. DOI: 10.1002/mana.200410340. URL: https://doi.org/10.1002/mana.200410340.

— (2007). "L_p estimates of solutions to mixed boundary value problems for the Stokes system in polyhedral domains". In: *Math. Nachr.* 280.7, pp. 751–793. ISSN: 0025-584X. DOI: 10.1002/mana.200610513. URL: https://doi.org/10.1002/mana.200610513.

— (2009). "Mixed boundary value problems for the stationary Navier-Stokes system in polyhedral domains". In: *Arch. Ration. Mech. Anal.* 194.2, pp. 669–712. ISSN: 0003-9527. DOI: 10.1007/s00205-008-0171-z. URL: https://doi.org/10.1007/s00205-008-0171-z.

Mohammadi, B. and O. Pironneau (1994). *Analysis of the k-epsilon turbulence model.* RAM: Research in Applied Mathematics. Masson, Paris; John Wiley & Sons, Ltd., Chichester, pp. xiv+196. ISBN: 2-225-84391-0.

Mohammadi, Bijan and Olivier Pironneau (2010). *Applied shape optimization for fluids*. Second. Numerical Mathematics and Scientific Computation. Oxford University Press, Oxford, pp. xiv+277. ISBN: 978-0-19-954690-9.

Moukalled, F., L. Mangani, and M. Darwish (2016). *The finite volume method in computational fluid dynamics*. Vol. 113. Fluid Mechanics and its Applications. An advanced introduction with OpenFOAM® and Matlab®. Springer, Cham, pp. xxiii+791. ISBN: 978-3-319-16873-9; 978-3-319-16874-6. DOI: 10.1007/978-3-319-16874-6. URL: https://doi.org/10.1007/978-3-319-16874-6.

Pantz, Olivier (2005). "Sensibilité de l'équation de la chaleur aux sauts de conductivité". In: *C. R. Math. Acad. Sci. Paris* 341.5, pp. 333–337. ISSN: 1631-073X. DOI: 10.1016/j.crma.2005.07.005. URL: https://doi.org/10.1016/j.crma.2005.07.005.

Pope, Stephen B. (2000). *Turbulent flows*. Cambridge University Press, Cambridge, pp. xxxiv+771. ISBN: 0-521-59886-9. DOI: 10.1017/CBO9780511840531. URL: https://doi.org/10.1017/CBO9780511840531.

Sokołowski, Jan and Jean-Paul Zolésio (1992). *Introduction to shape optimization*. Vol. 16. Springer Series in Computational Mathematics. Shape sensitivity analysis. Springer-Verlag, Berlin, pp. ii+250. ISBN: 3-540-54177-2. DOI: 10.1007/978-3-642-58106-9. URL: https://doi.org/10.1007/978-3-642-58106-9.

Sturm, Kevin (2015a). "On shape optimization with non-linear partial differential equations". PhD Thesis, Technischen Universität Berlin. PhD thesis, pp. vi+146.

— (2015b). "Shape differentiability under non-linear PDE constraints". In: *New trends in shape optimization*. Vol. 166. Internat. Ser. Numer. Math. Birkhäuser/Springer, Cham, pp. 271–300. DOI: 10.1007/978-3-319-17563-8_12. URL: https://doi.org/10.1007/978-3-319-17563-8_12.

Temam, Roger (2000). *Navier-Stokes equations. Theory and numerical analysis*. Studies in Mathematics and its Applications, Vol. 2. AMS Chelsea Publishing, p. 408. ISBN: 0-8218-2737-5.

Tröltzsch, Fredi (2010). *Optimal control of partial differential equations*. Vol. 112. Graduate Studies in Mathematics. Theory, methods and applications, Translated from the 2005 German original by Jürgen Sprekels. American Mathematical Society, Providence, RI, pp. xvi+399. ISBN: 978-0-8218-4904-0. DOI: 10.1090/gsm/112. URL: https://doi.org/10.1090/gsm/112.