S-6 Supplementary material

This section provides the transformations of the tangential gradient operator and unit normal vector, the first order variational of the related variables and transformed operators, the variational formulations of the related PDEs, the transformation of the related expressions, and the details for the adjoint analysis of the topology optimization problems.

S-6.1 Transformations of tangential gradient operator ∇_Γ and unit normal vector on Γ

The tangential gradient operator defined on a 2-manifold is the tangential component of the gradient operator defined in the 3D space in which the 2-manifold imbedded. Therefore, ∇_Γ can be transformed into

$$\begin{aligned}\nabla_\Gamma &= \mathbb{P}\nabla_{\mathbf{x}_\Xi} \\ &= \nabla_{\mathbf{x}_\Xi} - \left(\mathbf{n}_\Gamma \cdot \nabla_{\mathbf{x}_\Xi}\right)\mathbf{n}_\Gamma \\ &= \mathbb{T}_\Gamma^{-1}\nabla_{\mathbf{x}_\Omega} - \left[\mathbf{n}_\Gamma \cdot \left(\mathbb{T}_\Gamma^{-1}\nabla_{\mathbf{x}_\Omega}\right)\right]\mathbf{n}_\Gamma \\ &= \mathbb{T}_\Gamma^{-1}\left(\nabla_\Sigma + \nabla_\Sigma^\perp\right) - \left\{\mathbf{n}_\Gamma \cdot \left[\mathbb{T}_\Gamma^{-1}\left(\nabla_\Sigma + \nabla_\Sigma^\perp\right)\right]\right\}\mathbf{n}_\Gamma \\ &= \left\{\mathbb{T}_\Gamma^{-1}\nabla_\Sigma - \left[\mathbf{n}_\Gamma \cdot \left(\mathbb{T}_\Gamma^{-1}\nabla_\Sigma\right)\right]\mathbf{n}_\Gamma\right\} + \left\{\mathbb{T}_\Gamma^{-1}\nabla_\Sigma^\perp - \left[\mathbf{n}_\Gamma \cdot \left(\mathbb{T}_\Gamma^{-1}\nabla_\Sigma^\perp\right)\right]\mathbf{n}_\Gamma\right\},\end{aligned} \tag{S-63}$$

where $\mathbb{P}$ is the normal projector presented in Eq. 17; $\nabla_{\mathbf{x}_\Xi}$ and $\nabla_{\mathbf{x}_\Omega}$ are the gradient operators in the 3D Euclidean domains Ξ and Ω imbedded with Γ and Σ in the extended Cartesian systems of $\mathbf{x}_\Gamma$ and $\mathbf{x}_\Sigma$, respectively, and they satisfy $\nabla_{\mathbf{x}_\Xi} = \mathbb{T}_\Gamma^{-1}\nabla_{\mathbf{x}_\Omega}$ at $\mathbf{x}_\Gamma \in \Gamma$ with $\forall \mathbf{x}_\Sigma \in \Sigma$; and $\nabla_\Sigma^\perp$ is the normal component of $\nabla_{\mathbf{x}_\Sigma}$ on Σ. Because the variables on Σ are defined intrinsically, $\nabla_\Sigma^\perp$ is nonexistent. Therefore, the tangential gradient operator in Eq. S-63 can be transformed into Eq. 11. By implementing the dot product with $\mathbf{n}_\Gamma$ at the both sides of Eq. 11, $\mathbf{n}_\Gamma \cdot \nabla_\Gamma = 0$ can be retained for a differentiable function defined on Γ. Therefore, the transformed form of ∇_Γ in Eq. 11 is self-consistent.

From the relation in Eq. 6, the following geometrical relation among the unit normal vectors on Σ and Γ and the gradient of d_f can be derived as sketched in Fig. 2:

$$\mathbf{n}_\Gamma \parallel \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right),\ \forall \mathbf{x}_\Sigma \in \Sigma \tag{S-64}$$

where $\cdot \parallel \cdot$ represents the parallel relation of two vectors. Therefore, the unit normal vector on Γ can be derived by normalizing $\left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)$ at $\forall \mathbf{x}_\Sigma \in \Sigma$, i.e. the unit normal vector on Γ can be derived as Eq. 12.

S-6.2 First order variational of $\mathbf{n}_\Gamma^{(d_f)}$, $\nabla_\Gamma^{(d_f)}$ and $\mathrm{div}_\Gamma^{(d_f)}$ to d_f

The first order variational of the 2-norm of a vector function can be derived as

$$\delta\left(\|\mathbf{f}\|_2\right)^2 = 2\|\mathbf{f}\|_2\,\delta\|\mathbf{f}\|_2 = \delta\mathbf{f}^2 = 2\mathbf{f}\cdot\delta\mathbf{f} \Longrightarrow \delta\|\mathbf{f}\|_2 = \frac{\mathbf{f}}{\|\mathbf{f}\|_2}\cdot\delta\mathbf{f} \tag{S-65}$$

where $\mathbf{f}$ represents a vector function. Based on Eq. S-65, the first order variational of $\mathbf{n}_\Gamma^{(d_f)}$ to d_f can be derived as

$$\mathbf{n}_\Gamma^{(d_f;\tilde{d}_f)} = -\frac{\nabla_\Sigma\tilde{d}_f}{\|\mathbf{n}_\Sigma - \nabla_\Sigma d_f\|_2} + \frac{\mathbf{n}_\Gamma^{(d_f)}\cdot\nabla_\Sigma\tilde{d}_f}{\|\mathbf{n}_\Sigma - \nabla_\Sigma d_f\|_2}\mathbf{n}_\Gamma^{(d_f)},\ \forall\tilde{d}_f \in \mathcal{H}(\Sigma). \tag{S-66}$$

Because the tangential gradient operator ∇_Γ depends on d_f, its first-order variational to d_f can be derived as

$$\begin{aligned}\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}g =& \left(\frac{\partial\mathbb{T}_\Gamma^{-1}}{\partial d_f}\tilde{d}_{fa} + \frac{\partial\mathbb{T}_\Gamma^{-1}}{\partial\nabla_\Sigma d_f}\cdot\nabla_\Sigma\tilde{d}_{fa}\right)\nabla_\Sigma g - \left[\mathbf{n}_\Gamma^{(d_f;\tilde{d}_{fa})}\cdot\left(\mathbb{T}_\Gamma^{-1}\nabla_\Sigma g\right)\right]\mathbf{n}_\Gamma^{(d_f)} \\ &- \left\{\mathbf{n}_\Gamma^{(d_f)}\cdot\left[\left(\frac{\partial\mathbb{T}_\Gamma^{-1}}{\partial d_f}\tilde{d}_{fa} + \frac{\partial\mathbb{T}_\Gamma^{-1}}{\partial\nabla_\Sigma d_f}\cdot\nabla_\Sigma\tilde{d}_{fa}\right)\nabla_\Sigma g\right]\right\}\mathbf{n}_\Gamma^{(d_f)} \\ &- \left[\mathbf{n}_\Gamma^{(d_f)}\cdot\left(\mathbb{T}_\Gamma^{-1}\nabla_\Sigma g\right)\right]\mathbf{n}_\Gamma^{(d_f;\tilde{d}_{fa})}, \\ &\forall g \in \mathcal{H}(\Sigma)\ \text{and}\ \forall\tilde{d}_{fa} \in \mathcal{H}(\Sigma).\end{aligned} \tag{S-67}$$

Similarly, the first-order variational of div_Γ to d_f can be derived as

$$\begin{aligned}
\mathrm{div}_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{g} = \ & \mathrm{tr}\Bigg(\left(\frac{\partial \mathbb{T}_\Gamma^{-1}}{\partial d_f}\tilde{d}_{fa} + \frac{\partial \mathbb{T}_\Gamma^{-1}}{\partial \nabla_\Sigma d_f} \cdot \nabla_\Sigma \tilde{d}_{fa} \right) \nabla_\Sigma \mathbf{g} - \left[\mathbf{n}_\Gamma^{(d_f;\tilde{d}_{fa})} \cdot \left(\mathbb{T}_\Gamma^{-1} \nabla_\Sigma \mathbf{g} \right) \right] \mathbf{n}_\Gamma^{(d_f)} \\
& - \left\{ \mathbf{n}_\Gamma^{(d_f)} \cdot \left[\left(\frac{\partial \mathbb{T}_\Gamma^{-1}}{\partial d_f}\tilde{d}_{fa} + \frac{\partial \mathbb{T}_\Gamma^{-1}}{\partial \nabla_\Sigma d_f} \cdot \nabla_\Sigma \tilde{d}_{fa} \right) \nabla_\Sigma \mathbf{g} \right] \right\} \mathbf{n}_\Gamma^{(d_f)} \\
& - \left[\mathbf{n}_\Gamma^{(d_f)} \cdot \left(\mathbb{T}_\Gamma^{-1} \nabla_\Sigma \mathbf{g} \right) \right] \mathbf{n}_\Gamma^{(d_f;\tilde{d}_{fa})} \Bigg), \\
& \forall \mathbf{g} \in \left(\mathcal{H}(\Sigma)\right)^3 \ \text{and} \ \forall \tilde{d}_{fa} \in \mathcal{H}(\Sigma).
\end{aligned} \tag{S-68}$$

Because d_f is a differentiable homeomorphism, it can induce the Riemannian metric for Γ. Then, the differential on the base manifold and implicit 2-manifold satisfies

$$\begin{cases} \mathrm{d}\Gamma = |\mathbb{T}_\Gamma| \left\| \mathbb{T}_\Gamma \mathbf{n}_\Gamma^{(d_f)} \right\|_2^{-1} \mathrm{d}\Sigma \\ \mathrm{d}l_{\partial\Gamma} = \|\boldsymbol{\tau}_\Gamma\|_2 \left\| \mathbb{T}_\Gamma^{-1} \boldsymbol{\tau}_\Gamma \right\|_2^{-1} \mathrm{d}l_{\partial\Sigma} \end{cases}, \tag{S-69}$$

where $\mathrm{d}l_{\partial\Gamma}$ and $\mathrm{d}l_{\partial\Sigma}$ are the differential of the boundary curves of Γ and Σ, respectively. In Eq. S-69, the unit tangential vector $\boldsymbol{\tau}_\Gamma$ at $\partial\Gamma$ sketched in Fig. 2 satisfies

$$\left. \begin{aligned} & \mathbf{n}_{\boldsymbol{\tau}_\Sigma} \parallel (\mathbf{n}_\Sigma \times \nabla_\Sigma d_f) \\ & \mathbf{n}_\Gamma \parallel (\mathbf{n}_\Sigma - \nabla_\Sigma d_f) \\ & \mathbf{n}_{\boldsymbol{\tau}_\Gamma} = \mathbf{n}_\Gamma \times \boldsymbol{\tau}_\Gamma \\ & \boldsymbol{\tau}_\Sigma \parallel \nabla_\Sigma d_f \end{aligned} \right\} \Rightarrow \boldsymbol{\tau}_\Gamma \parallel \left[(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f) \times (\mathbf{n}_\Sigma - \nabla_\Sigma d_f) \right]. \tag{S-70}$$

Therefore, the second equation in Eq. S-69 can be transformed into

$$\mathrm{d}l_{\partial\Gamma} = \left\| (\mathbf{n}_\Sigma \times \nabla_\Sigma d_f) \times (\mathbf{n}_\Sigma - \nabla_\Sigma d_f) \right\|_2 \left\| \mathbb{T}_\Gamma^{-1} \left[(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f) \times (\mathbf{n}_\Sigma - \nabla_\Sigma d_f) \right] \right\|_2^{-1} \mathrm{d}l_{\partial\Sigma}. \tag{S-71}$$

In the following parts, $M^{(d_f)}$ and $L^{(d_f)}$ for Eqs. S-69 and S-71 are derived as

$$\begin{cases} M^{(d_f)} \doteq |\mathbb{T}_\Gamma| \left\| \mathbb{T}_\Gamma \mathbf{n}_\Gamma^{(d_f)} \right\|_2^{-1} \\ L^{(d_f)} \doteq \left\| (\mathbf{n}_\Sigma \times \nabla_\Sigma d_f) \times (\mathbf{n}_\Sigma - \nabla_\Sigma d_f) \right\|_2 \left\| \mathbb{T}_\Gamma^{-1} \left[(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f) \times (\mathbf{n}_\Sigma - \nabla_\Sigma d_f) \right] \right\|_2^{-1} \end{cases}. \tag{S-72}$$

S-6.3 Variational formulations of surface-PDE filters

The variational formulation of the surface-PDE filter in Eq. 5 is considered in the first order Sobolev space defined on Σ. It can be derived based on the Galerkin method:

$$\begin{cases} \text{Find } d_f \in \mathcal{H}(\Sigma) \ \text{for } d_m \in \mathcal{L}^2(\Sigma) \ \text{and } \forall \tilde{d}_f \in \mathcal{H}(\Sigma), \\ \text{such that } \displaystyle\int_\Sigma r_m^2 \nabla_\Sigma d_f \cdot \nabla_\Sigma \tilde{d}_f + d_f \tilde{d}_f - A_d \left(d_m - \frac{1}{2} \right) \tilde{d}_f \, \mathrm{d}\Sigma = 0 \end{cases} \tag{S-73}$$

where $\tilde{d}_f$ is the test function of d_f; $\mathcal{H}(\Sigma)$ represents the first order Sobolev space defined on Σ; and $\mathcal{L}^2(\Sigma)$ represents the second order Lebesque space defined on Σ.

The variational formulation of the surface-PDE filter in Eq. 9 is considered in the first order Sobolev space defined on Γ_D. It can be derived based on the Galerkin method:

$$\begin{cases} \text{Find } \gamma_f \in \mathcal{H}(\Gamma_D) \ \text{for } \gamma \in \mathcal{L}^2(\Gamma_D) \ \text{and } \forall \tilde{\gamma}_f \in \mathcal{H}(\Gamma_D), \\ \text{such that } \displaystyle\int_{\Gamma_D} r_f^2 \nabla_\Gamma \gamma_f \cdot \nabla_\Gamma \tilde{\gamma}_f + \gamma_f \tilde{\gamma}_f - \gamma \tilde{\gamma}_f \, \mathrm{d}\Gamma = 0 \end{cases} \tag{S-74}$$

where $\tilde{\gamma}_f$ is the test function of γ_f; $\mathcal{H}(\Gamma_D)$ represents the first order Sobolev space defined on Γ_D; and $\mathcal{L}^2(\Gamma_D)$ represents the second order Lebesque space defined on Γ_D.

Based on the transformed tangential gradient operator in Eq. 13, the homeomorphism between $\mathcal{H}(\Gamma)$ and $\mathcal{H}(\Sigma)$ described in Eq. 6 and the homeomorphism between $\mathcal{H}(\Gamma_D)$ and $\mathcal{H}(\Sigma_D)$ described in Eq. 7, the coupling relation between the two sets of design variables can be derived by instituting Eq. 13 into Eq. S-74:

$$\begin{cases} \text{Find } \gamma_f \in \mathcal{H}(\Sigma_D) \ \text{for } \gamma \in \mathcal{L}^2(\Sigma_D) \ \text{and } \forall \tilde{\gamma}_f \in \mathcal{H}(\Sigma_D), \\ \text{such that } \displaystyle\int_{\Sigma_D} \left(r_f^2 \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f)} \tilde{\gamma}_f + \gamma_f \tilde{\gamma}_f - \gamma \tilde{\gamma}_f \right) M^{(d_f)} \, \mathrm{d}\Sigma = 0 \end{cases} \tag{S-75}$$

where the tangential gradient operator ∇_Γ on Γ is replaced by its transformed form $\nabla_\Gamma^{(d_f)}$ in Eq. 13; and $\mathcal{H}(\Sigma_D)$ and $\mathcal{L}^2(\Sigma_D)$ defined on Σ_D are the homeomorphous counterparts of $\mathcal{H}(\Gamma_D)$ and $\mathcal{L}^2(\Gamma_D)$, respectively.

S-6.4 Variational formulation of surface Navier-Stokes equations

The variational formulation of the surface Navier-Stokes equations is considered in the functional spaces without containing the tangential constraint of the fluid velocity. The tangential constraint of the fluid velocity is imposed by using the Lagrangian multiplier [1, 2]. Based on the Galerkin method, the variational formulation of the surface Navier-Stokes equations can be derived as

$$\left\{\begin{aligned} &\text{Find}\left\{\begin{aligned} &\mathbf{u}\in\left(\mathcal{H}\left(\Gamma\right)\right)^3 \text{ with } \left\{\begin{aligned} &\mathbf{u}=\mathbf{u}_{l_{v,\Gamma}} \text{ at } \forall\mathbf{x}_\Gamma\in l_{v,\Gamma}\\ &\mathbf{u}=\mathbf{0} \text{ at } \forall\mathbf{x}_\Gamma\in l_{v_0,\Gamma}\end{aligned}\right.\\ &p\in\mathcal{H}\left(\Gamma\right)\\ &\lambda\in\mathcal{L}^2\left(\Gamma\right) \text{ with } \lambda=0 \text{ at } \forall\mathbf{x}_\Gamma\in l_{v,\Gamma}\cup l_{v_0,\Gamma}\end{aligned}\right.\\ &\text{for}\left\{\begin{aligned} &\forall\tilde{\mathbf{u}}\in\left(\mathcal{H}\left(\Gamma\right)\right)^3\\ &\forall\tilde{p}\in\mathcal{H}\left(\Gamma\right)\\ &\forall\tilde{\lambda}\in\mathcal{L}^2\left(\Gamma\right)\end{aligned}\right., \text{ such that}\\ &\int_\Gamma \rho\left(\mathbf{u}\cdot\nabla_\Gamma\right)\mathbf{u}\cdot\tilde{\mathbf{u}}+\frac{\eta}{2}\left(\nabla_\Gamma\mathbf{u}+\nabla_\Gamma\mathbf{u}^\mathrm{T}\right):\left(\nabla_\Gamma\tilde{\mathbf{u}}+\nabla_\Gamma\tilde{\mathbf{u}}^\mathrm{T}\right)-p\,\mathrm{div}_\Gamma\tilde{\mathbf{u}}-\tilde{p}\,\mathrm{div}_\Gamma\mathbf{u}\\ &+\alpha\mathbf{u}\cdot\tilde{\mathbf{u}}+\lambda\tilde{\mathbf{u}}\cdot\mathbf{n}_\Gamma+\tilde{\lambda}\mathbf{u}\cdot\mathbf{n}_\Gamma\,\mathrm{d}\Gamma-\sum_{E_\Gamma\in\mathcal{E}_\Gamma}\int_{E_\Gamma}\tau_{BP,\Gamma}\nabla_\Gamma p\cdot\nabla_\Gamma\tilde{p}\,\mathrm{d}\Gamma=0\end{aligned}\right. \tag{S-76}$$

where λ is the Lagrange multiplier used to impose the tangential constraint of the fluid velocity; $\tilde{\mathbf{u}}$, $\tilde{p}$ and $\tilde{\lambda}$ are the test functions of $\mathbf{u}$, p and λ, respectively; the Brezzi-Pitkäranta stabilization term

$$-\sum_{E_\Gamma\in\mathcal{E}_\Gamma}\int_{E_\Gamma}\tau_{BP,\Gamma}\nabla_\Gamma p\cdot\nabla_\Gamma\tilde{p}\,\mathrm{d}\Gamma \tag{S-77}$$

with $\tau_{BP,\Gamma}$ representing the stabilization parameter is imposed on the variational formulation, in order to use linear finite elements to solve both the fluid velocity and pressure; $\mathcal{E}_\Gamma$ is an elementization of Γ; and E_Γ is an element of the elementization $\mathcal{E}_\Gamma$. The stabilization parameter is chosen as [3]

$$\tau_{BP,\Gamma}=\frac{h_{E_\Gamma}^2}{12\eta}, \tag{S-78}$$

where h_{E_Γ} is the size of the element E_Γ. Because the element E_Γ and the elementization $\mathcal{E}_\Gamma$ for the 2-manifold Γ are implicitly defined on the base manifold Σ, they are derived from the design variable for the implicit 2-manifold Γ and the explicit elementization $\mathcal{E}_\Sigma$ of the base manifold Σ. Based on Eqs. S-69 and S-72, $h_{E_\Gamma}^2$ in $\tau_{BP,\Gamma}$ can be approximated by the area of E_Γ. Then, it can be transformed into

$$\begin{aligned} h_{E_\Gamma}^2 &\approx \int_{E_\Gamma} 1\,\mathrm{d}\Gamma\\ &=\int_{E_\Sigma} M^{(d_f)}\,\mathrm{d}\Sigma\\ &\approx h_{E_\Sigma}^2\int_{E_\Sigma} M^{(d_f)}\,\mathrm{d}\Sigma\Big/\int_{E_\Sigma} 1\,\mathrm{d}\Sigma\\ &=h_{E_\Sigma}^2\bar{M}_{E_\Sigma}^{(d_f)}, \end{aligned} \tag{S-79}$$

where h_{E_Σ} is the size of the element E_Σ representing an element of the explicit elementization $\mathcal{E}_\Sigma$ of Σ; $\bar{M}_{E_\Sigma}^{(d_f)}$ is the average value of $M^{(d_f)}$ in the element E_Σ; and the area of E_Σ can be approximated as $h_{E_\Sigma}^2$, i.e. $\int_{E_\Sigma} 1\,\mathrm{d}\Sigma\approx h_{E_\Sigma}^2$. Because the elementization satisfies $h_{E_\Sigma}^2\ll|\Sigma|$ with $|\Sigma|$ representing the area of Σ, $\bar{M}_{E_\Sigma}^{(d_f)}$ can be well approximated by the value of $M^{(d_f)}$ at $\forall\mathbf{x}_\Sigma\in E_\Sigma$, i.e.

$$\bar{M}_{E_\Sigma}^{(d_f)}\approx M^{(d_f)},\ \forall\mathbf{x}_\Sigma\in E_\Sigma. \tag{S-80}$$

Therefore, the stabilization parameter $\tau_{BP,\Gamma}$ in Eq. S-78 can be transformed into

$$\tau_{BP,\Gamma}^{(d_f)}=\frac{h_{E_\Sigma}^2}{12\eta}M^{(d_f)}. \tag{S-81}$$

Because $l_{v,\Gamma}$ and $l_{v_0,\Gamma}$ are homeomorphous to $l_{v,\Sigma}$ and $l_{v_0,\Sigma}$, respectively, $l_{v,\Sigma}$ and $l_{v_0,\Sigma}$ are fixed, and $\mathbf{u}_{l_{v,\Gamma}}$ is homeomorphous to $\mathbf{u}_{l_{v,\Sigma}}$, the variational formulation in Eq. S-76 can be transformed into the following form defined on Σ based on the coupling relations in Section

2.2.3:

$$\begin{cases} \text{Find} \begin{cases} \mathbf{u} \in (\mathcal{H}(\Sigma))^3 \text{ with } \begin{cases} \mathbf{u} = \mathbf{u}_{l_{v,\Sigma}} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \\ \mathbf{u} = \mathbf{0} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v_0,\Sigma} \end{cases} \\ p \in \mathcal{H}(\Sigma) \\ \lambda \in \mathcal{L}^2(\Sigma) \text{ with } \lambda = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \end{cases} \\ \text{for} \begin{cases} \forall \tilde{\mathbf{u}} \in (\mathcal{H}(\Sigma))^3 \\ \forall \tilde{p} \in \mathcal{H}(\Sigma) \\ \forall \tilde{\lambda} \in \mathcal{L}^2(\Sigma) \end{cases}, \text{ such that} \\ \int_\Sigma \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \mathbf{u} \cdot \tilde{\mathbf{u}} + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}} + \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}^\mathrm{T} \right) \right. \\ \left. - p \,\mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}} - \tilde{p} \,\mathrm{div}_\Gamma^{(d_f)} \mathbf{u} + \alpha \mathbf{u} \cdot \tilde{\mathbf{u}} + \lambda \tilde{\mathbf{u}} \cdot \mathbf{n}_\Gamma^{(d_f)} + \tilde{\lambda} \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} \right] M^{(d_f)} \,\mathrm{d}\Sigma \\ - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{BP,\Gamma}^{(d_f)} \nabla_\Gamma^{(d_f)} p \cdot \nabla_\Gamma^{(d_f)} \tilde{p} M^{(d_f)} \,\mathrm{d}\Sigma = 0. \end{cases} \tag{S-82}$$

S-6.5 Variational formulation of surface convection-diffusion equation

Based on the Galerkin method, the variational formulation of the surface convection-diffusion equation is considered in the first order Sobolev space defined on the implicit 2-manifold Γ:

$$\begin{cases} \text{Find } c \in \mathcal{H}(\Gamma) \text{ with } c = c_0 \text{ at } \forall \mathbf{x}_\Gamma \in l_{v,\Gamma}, \text{ for } \forall \tilde{c} \in \mathcal{H}(\Gamma), \text{ such that} \\ \int_\Gamma (\mathbf{u} \cdot \nabla_\Gamma c) \tilde{c} + D \nabla_\Gamma c \cdot \nabla_\Gamma \tilde{c} \,\mathrm{d}\Gamma + \sum_{E_\Gamma \in \mathcal{E}_\Gamma} \int_{E_\Gamma} \tau_{PG,\Gamma} (\mathbf{u} \cdot \nabla_\Gamma c) (\mathbf{u} \cdot \nabla_\Gamma \tilde{c}) \,\mathrm{d}\Gamma = 0 \end{cases} \tag{S-83}$$

where $\tilde{c}$ is the test function of c; the Petrov-Galerkin stabilization term

$$\sum_{E_\Gamma \in \mathcal{E}_\Gamma} \int_{E_\Gamma} \tau_{PG,\Gamma} (\mathbf{u} \cdot \nabla_\Gamma c) (\mathbf{u} \cdot \nabla_\Gamma \tilde{c}) \,\mathrm{d}\Gamma \tag{S-84}$$

with $\tau_{PG,\Gamma}$ representing the stabilization parameter is imposed on the variational formulation, in order to use the linear finite elements to solve the distribution of the concentration. The stabilization parameter is chosen as [3]

$$\tau_{PG,\Gamma} = \left(\frac{4}{h_{E_\Gamma}^2 D} + \frac{2 \|\mathbf{u}\|_2}{h_{E_\Gamma}} \right)^{-1}. \tag{S-85}$$

Based on Eqs. S-69, S-79 and S-80, $\tau_{PG,\Gamma}$ can be transformed into

$$\tau_{PG,\Gamma}^{(d_f)} = \left(\frac{4}{h_{E_\Sigma}^2 M^{(d_f)} D} + \frac{2 \|\mathbf{u}\|_2}{h_{E_\Sigma} \left(M^{(d_f)} \right)^{\frac{1}{2}}} \right)^{-1}. \tag{S-86}$$

Based on the homeomorphisms and the coupling relations in Section 2.2.3, the variational formulation in Eq. S-83 can be transformed into the form defined on Σ:

$$\begin{cases} \text{Find } c \in \mathcal{H}(\Sigma) \text{ with } c = c_0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma}, \text{ for } \forall \tilde{c} \in \mathcal{H}(\Sigma), \\ \text{such that } \int_\Sigma \left[\left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} c \right) \tilde{c} + D \nabla_\Gamma^{(d_f)} c \cdot \nabla_\Gamma^{(d_f)} \tilde{c} \right] M^{(d_f)} \,\mathrm{d}\Sigma \\ + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{PG,\Gamma}^{(d_f)} \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{c} \right) M^{(d_f)} \,\mathrm{d}\Sigma = 0. \end{cases} \tag{S-87}$$

S-6.6 Transformation of design objective in Eq. 21 and pressure drop in Eq. 23

Based on the coupling relations in Section 2.2.3 and Eq. S-72, the design objective in Eq. 21 can be transformed into

$$J_c^{(d_f)} = \int_{l_{s,\Sigma}} (c - \bar{c})^2 L^{(d_f)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} (c_0 - \bar{c})^2 L^{(d_f)} \,\mathrm{d}l_{\partial\Sigma}. \tag{S-88}$$

Based on Eq. S-72 and the relation in Eq. S-70 sketched in Fig. 2, the pressure drop in Eq. 23 can be transformed into

$$\Delta P^{(d_f)} = \int_{l_{v,\Sigma}} p L^{(d_f)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} p L^{(d_f)} \,\mathrm{d}l_{\partial\Sigma}. \tag{S-89}$$

S-6.7 Variational formulations of adjoint equations for design objective in Eq. 21

The variational formulation for the adjoint equation of the surface convection-diffusion equation is derived as

$$\left\{\begin{aligned} & \text{Find } c_a \in \mathcal{H}\left(\Sigma\right) \text{ with } c_a = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma}, \text{ for } \forall \tilde{c}_a \in \mathcal{H}\left(\Sigma\right) \\ & \text{such that } \int_{l_{s,\Sigma}} 2\left(c-\bar{c}\right) L^{\left(d_f\right)} \tilde{c}_a \,\mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} \left(c_0-\bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\ & + \int_\Sigma \left[\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\tilde{c}_a\right) c_a + D\nabla_\Gamma^{\left(d_f\right)}\tilde{c}_a \cdot \nabla_\Gamma^{\left(d_f\right)} c_a\right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma \\ & + \sum_{E_\Sigma\in\mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\tilde{c}_a\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right) M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0 \end{aligned}\right. \tag{S-90}$$

where c_a is the adjoint variable of c and $\tilde{c}_a$ is the test function of c_a. The variational formulation for the adjoint equations of the surface Naiver-Stokes equations is derived as

$$\left\{\begin{aligned} & \text{Find} \left\{\begin{aligned} & \mathbf{u}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \text{ with } \mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\ & p_a \in \mathcal{H}\left(\Sigma\right) \\ & \lambda_a \in \mathcal{L}^2\left(\Sigma\right) \text{ with } \lambda_a = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \end{aligned}\right. \\ & \text{for} \left\{\begin{aligned} & \forall \tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\ & \forall \tilde{p}_a \in \mathcal{H}\left(\Sigma\right) \\ & \forall \tilde{\lambda}_a \in \mathcal{L}^2\left(\Sigma\right) \end{aligned}\right. , \text{ such that} \\ & \int_\Sigma \left[\rho\left(\tilde{\mathbf{u}}_a\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\tilde{\mathbf{u}}_a\cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\tilde{\mathbf{u}}_a + \nabla_\Gamma^{\left(d_f\right)}\tilde{\mathbf{u}}_a^\mathrm{T}\right)\right. \\ & : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) - \tilde{p}_a \mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a - p_a \mathrm{div}_\Gamma^{\left(d_f\right)}\tilde{\mathbf{u}}_a + \alpha\tilde{\mathbf{u}}_a\cdot\mathbf{u}_a + \left(\tilde{\lambda}_a\mathbf{u}_a + \lambda_a\tilde{\mathbf{u}}_a\right) \\ & \left.\cdot\,\mathbf{n}_\Gamma^{\left(d_f\right)} + \left(\tilde{\mathbf{u}}_a\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)c_a\right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma + \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\left[-\tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}\tilde{p}_a\cdot\nabla_\Gamma^{\left(d_f\right)}p_a\right. \\ & + \tau_{PG,\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right) + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\tilde{\mathbf{u}}_a\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right) \\ & \left. + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\tilde{\mathbf{u}}_a\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right)\right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0 \end{aligned}\right. \tag{S-91}$$

where $\mathbf{u}_a$, p_a and λ_a are the adjoint variables of $\mathbf{u}$, p and λ, respectively; $\tilde{\mathbf{u}}_a$, $\tilde{p}_a$ and $\tilde{\lambda}_a$ are the test functions of $\mathbf{u}_a$, p_a and λ_a, respectively; and $\tau_{PG,\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)}$ is the first-order variational of $\tau_{PG,\Gamma}^{\left(d_f\right)}$ to $\mathbf{u}$, and it is expressed as

$$\tau_{PG,\Gamma}^{\left(d_f,\tilde{\mathbf{u}}_a\right)} = -\left(\frac{4}{h_{E_\Sigma}^2 M^{\left(d_f\right)} D} + \frac{2\left\|\mathbf{u}\right\|_2}{h_{E_\Sigma}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}}\right)^{-2} \frac{2\mathbf{u}\cdot\tilde{\mathbf{u}}_a}{h_{E_\Sigma}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}\left\|\mathbf{u}\right\|_2}, \ \forall\tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3. \tag{S-92}$$

The variational formulations for the adjoint equations of the surface-PDE filters for γ and d_m are derived as

$$\left\{\begin{aligned} & \text{Find } \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \text{ for } \forall\tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right), \text{ such that} \\ & \int_{\Sigma_D}\left(\frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\mathbf{u}_a\tilde{\gamma}_{fa} + r_f^2\nabla_\Gamma^{\left(d_f\right)}\tilde{\gamma}_{fa}\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \tilde{\gamma}_{fa}\gamma_{fa}\right) M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0 \end{aligned}\right. \tag{S-93}$$

and

$$\begin{cases}\text{Find } d_{fa} \in \mathcal{H}(\Sigma) \text{ for } \forall \tilde{d}_{fa} \in \mathcal{H}(\Sigma), \text{ such that} \\ \int_{l_{s,\Sigma}} (c-\bar{c})^2 L^{\left(d_f;\tilde{d}_{fa}\right)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} (c_0-\bar{c})^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} (c-\bar{c})^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\ \int_{l_{v,\Sigma}} (c_0-\bar{c})^2 L^{\left(d_f;\tilde{d}_{fa}\right)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \left(\int_{l_{v,\Sigma}} (c_0-\bar{c})^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma}\right)^2 + \int_\Sigma \left[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\right)\mathbf{u}\right. \\ \cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) \\ : \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\mathbf{u} + (\lambda\mathbf{u}_a + \lambda_a\mathbf{u}) \\ \cdot\mathbf{n}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} + \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}c\right)c_a + D\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}c\cdot\nabla_\Gamma^{\left(d_f\right)}c_a + D\nabla_\Gamma^{\left(d_f\right)}c\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}c_a \\ + f_{id,\Gamma}r_f^2\left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \nabla_\Gamma^{\left(d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\gamma_{fa}\right)\Big]M^{\left(d_f\right)} + \left[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\right. \\ \cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u} \\ + \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)c_a + D\nabla_\Gamma^{\left(d_f\right)}c\cdot\nabla_\Gamma^{\left(d_f\right)}c_a \\ + f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right)\Big]M^{\left(d_f;\tilde{d}_{fa}\right)} \\ + r_m^2\nabla_\Sigma\tilde{d}_{fa}\cdot\nabla_\Sigma d_{fa} + \tilde{d}_{fa}d_{fa}\,\mathrm{d}\Sigma \\ + \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\left[\left(-\tau_{BP,\Gamma}^{\left(d_f;\tilde{d}_f\right)}\nabla_\Gamma^{\left(d_f\right)}p\cdot\nabla_\Gamma^{\left(d_f\right)}p_a - \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}p\cdot\nabla_\Gamma^{\left(d_f\right)}p_a - \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}p\right.\right. \\ \left.\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}p_a\right) + \tau_{PG,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right) + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}c\right) \\ \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right) + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}c_a\right)\Big]M^{\left(d_f\right)} + \Big[-\tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}p \\ \cdot\nabla_\Gamma^{\left(d_f\right)}p_a + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right)\Big]M^{\left(d_f;\tilde{d}_{fa}\right)}\,\mathrm{d}\Sigma = 0\end{cases} \tag{S-94}$$

where $\tilde{\gamma}_{fa}$ and $\tilde{d}_{fa}$ are the test functions of γ_{fa} and d_{fa}, respectively; $\tau_{BP,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)}$ and $\tau_{PG,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)}$ are the first-order variationals of $\tau_{BP,\Gamma}^{\left(d_f\right)}$ and $\tau_{PG,\Gamma}^{\left(d_f\right)}$ to d_f, respectively, and they are expressed as

$$\tau_{BP,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} = \frac{h_{E_\Sigma}^2}{12\eta}M^{\left(d_f;\tilde{d}_{fa}\right)},\ \forall\tilde{d}_{fa}\in\mathcal{H}(\Sigma) \tag{S-95}$$

and

$$\begin{split}\tau_{PG,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} = & \left(\frac{4}{h_{E_\Sigma}^2 M^{\left(d_f\right)}D} + \frac{2\left\|\mathbf{u}\right\|_2}{h_{E_\Sigma}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}}\right)^{-2} \\ & \left(\frac{4}{h_{E_\Sigma}^2\left(M^{\left(d_f\right)}\right)^2 D} + \frac{\left\|\mathbf{u}\right\|_2}{h_{E_\Sigma}\left(M^{\left(d_f\right)}\right)^{\frac{3}{2}}}\right)M^{\left(d_f;\tilde{d}_{fa}\right)},\ \forall\tilde{d}_f\in\mathcal{H}(\Sigma);\end{split} \tag{S-96}$$

$M^{\left(d_f;\tilde{d}_{fa}\right)}$ and $L^{\left(d_f;\tilde{d}_{fa}\right)}$ are the first-order variationals of $M^{\left(d_f\right)}$ and $L^{\left(d_f\right)}$ to d_f derived based on Eq. 8 and Eq. S-65 in the supplementary material, and they are expressed as

$$\begin{split}M^{\left(d_f;\tilde{d}_{fa}\right)} = & \left(\frac{\partial\left|\mathbb{T}_\Gamma\right|}{\partial d_f}\tilde{d}_{fa} + \frac{\partial\left|\mathbb{T}_\Gamma\right|}{\partial\nabla_\Sigma d_f}\cdot\nabla_\Sigma\tilde{d}_{fa}\right)\left\|\mathbb{T}_\Gamma\mathbf{n}_\Gamma^{\left(d_f\right)}\right\|_2^{-1} - \left|\mathbb{T}_\Gamma\right|\left\|\mathbb{T}_\Gamma\mathbf{n}_\Gamma^{\left(d_f\right)}\right\|_2^{-3} \\ & \left[\frac{\partial\mathbb{T}_\Gamma}{\partial d_f}\mathbf{n}_\Gamma^{\left(d_f\right)}\tilde{d}_{fa} + \left(\frac{\partial\mathbb{T}_\Gamma}{\partial\nabla_\Sigma d_f}\cdot\nabla_\Sigma\tilde{d}_{fa}\right)\mathbf{n}_\Gamma^{\left(d_f\right)} + \mathbb{T}_\Gamma\mathbf{n}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\right] \\ & \cdot\left(\mathbb{T}_\Gamma\mathbf{n}_\Gamma^{\left(d_f\right)}\right),\ \forall\tilde{d}_{fa}\in\mathcal{H}(\Sigma)\end{split} \tag{S-97}$$

and

$$
\begin{split}
L^{\left(d_f;\tilde{d}_{fa}\right)} = & \frac{\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)}{\left\|\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right\|_2} \cdot \left[\frac{\partial\left[\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right]}{\nabla_\Sigma d_f} \cdot \nabla_\Sigma \tilde{d}_{fa} \right] \\
& \left\|\mathbb{T}_\Gamma^{-1} \left[\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right]\right\|_2^{-1} + \left\|\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right\|_2 \\
& \left\|\mathbb{T}_\Gamma^{-1} \left[\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right]\right\|_2^{-3} \left\{ \left(\frac{\partial \mathbb{T}_\Gamma^{-1}}{\partial d_f} \tilde{d}_{fa} + \frac{\partial \mathbb{T}_\Gamma^{-1}}{\partial \nabla_\Sigma d_f} \cdot \nabla_\Sigma \tilde{d}_{fa} \right) \right. \\
& \left[\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right] + \mathbb{T}_\Gamma^{-1} \left[\frac{\partial\left[\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right]}{\partial \nabla_\Sigma d_f} \right. \\
& \left. \left. \cdot \nabla_\Sigma \tilde{d}_{fa} \right] \right\} \cdot \left\{ \mathbb{T}_\Gamma^{-1} \left[\left(\mathbf{n}_\Sigma \times \nabla_\Sigma d_f\right) \times \left(\mathbf{n}_\Sigma - \nabla_\Sigma d_f\right)\right] \right\}, \ \forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right).
\end{split} \tag{S-98}
$$

S-6.8 Adjoint analysis for design objective in Eq. 24

Based on the transformed design objective in Eq. S-88, the variational formulations of the surface-PDE filters in Eqs. S-73 and S-74, the surface Navier-Stokes equations in Eq. S-82 and the surface convection-diffusion equation in Eq. S-87, the augmented Lagrangian of the design objective in Eq. 24 can be derived as

$$
\begin{split}
\hat{J}_c = & \int_{l_{s,\Sigma}} \left(c - \bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} \left(c_0 - \bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} + \int_\Sigma \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \right) \mathbf{u} \cdot \mathbf{u}_a \right. \\
& + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T} \right) - p \,\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} \\
& \left. + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} \right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} p \\
& \cdot \nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)} \,\mathrm{d}\Sigma + \int_\Gamma \left[\left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) c_a + D \nabla_\Gamma^{\left(d_f\right)} c \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma \\
& + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) M^{\left(d_f\right)} \,\mathrm{d}\Sigma + \int_\Sigma f_{id,\Gamma} \\
& \left(r_f^2 \nabla_\Gamma^{\left(d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa} \right) M^{\left(d_f\right)} + r_m^2 \nabla_\Sigma d_f \cdot \nabla_\Sigma d_{fa} \\
& + d_f d_{fa} - A_d \left(d_m - \frac{1}{2} \right) d_{fa} \,\mathrm{d}\Sigma,
\end{split} \tag{S-99}
$$

where $\hat{J}_c$ is the augmented lagrangian of J_c; and the adjoint variables satisfy

$$
\left.\begin{aligned}
& \mathbf{u}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\
& p_a \in \mathcal{H}\left(\Sigma\right) \\
& \lambda_a \in \mathcal{L}^2\left(\Sigma\right) \\
& c_a \in \mathcal{H}\left(\Sigma\right) \\
& \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \\
& d_{fa} \in \mathcal{H}\left(\Sigma\right)
\end{aligned}\right\} \text{ with } \begin{cases}
\mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\
\lambda_a = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\
c_a = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma}
\end{cases}. \tag{S-100}
$$

Based on the transformed operators in Eqs. 13 and 14 and their first order variationals in Eqs. S-67 and S-68, together with the first order variational of the 2-norm of a vector function in Eq. S-65, the first order variational of the augmented Lagrangian in Eq. S-99 can be derived as

$$
\begin{aligned}
\delta \hat{J}_c = & \int_{l_{s,\Sigma}} \left[2\left(c-\bar{c}\right) L^{\left(d_f\right)} \delta c + \left(c-\bar{c}\right)^2 L^{\left(d_f;\delta d_f\right)} \right] \mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} \left(c_0-\bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\
& - \int_{l_{s,\Sigma}} \left(c-\bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \int_{l_{v,\Sigma}} \left(c_0-\bar{c}\right)^2 L^{\left(d_f;\delta d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \left(\int_{l_{v,\Sigma}} \left(c_0-\bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \right)^2 \\
& + \int_\Sigma \bigg[\rho \left(\delta\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\delta\mathbf{u}\cdot\mathbf{u}_a + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a \\
& + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\delta\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\delta\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}^\mathrm{T}\right) \\
& : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}_a^\mathrm{T}\right) \\
& - \delta p \,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a - p\,\mathrm{div}_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u} - p_a\mathrm{div}_\Gamma^{\left(d_f\right)}\delta\mathbf{u} + \alpha\delta\mathbf{u}\cdot\mathbf{u}_a \\
& + \frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\mathbf{u}_a\delta\gamma_f + \left(\lambda\mathbf{u}_a + \lambda_a\mathbf{u}\right)\cdot\mathbf{n}_\Gamma^{\left(d_f;\delta d_f\right)} + \left(\delta\lambda\mathbf{u}_a + \lambda_a\delta\mathbf{u}\right)\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} \bigg] M^{\left(d_f\right)} \\
& + \bigg[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) \\
& - p\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u} + \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f\right)}\bigg] M^{\left(d_f;\delta d_f\right)} \,\mathrm{d}\Sigma \\
& - \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma} \tau_{BP,\Gamma}^{\left(d_f;\delta d_f\right)}\nabla_\Gamma^{\left(d_f\right)}p\cdot\nabla_\Gamma^{\left(d_f\right)}p_a M^{\left(d_f\right)} + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}\delta p\cdot\nabla_\Gamma^{\left(d_f\right)}p_a M^{\left(d_f\right)} \\
& + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f;\delta d_f\right)}p\cdot\nabla_\Gamma^{\left(d_f\right)}p_a M^{\left(d_f\right)} + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}p\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}p_a M^{\left(d_f\right)} \\
& + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}p\cdot\nabla_\Gamma^{\left(d_f\right)}p_a M^{\left(d_f;\delta d_f\right)} \,\mathrm{d}\Sigma + \int_\Sigma \bigg[\left(\delta\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)c_a + \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\delta c\right)c_a \\
& + \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}c\right)c_a + D\nabla_\Gamma^{\left(d_f\right)}\delta c\cdot\nabla_\Gamma^{\left(d_f\right)}c_a + D\nabla_\Gamma^{\left(d_f;\delta d_f\right)}c\cdot\nabla_\Gamma^{\left(d_f\right)}c_a + D\nabla_\Gamma^{\left(d_f\right)}c \\
& \cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}c_a\bigg] M^{\left(d_f\right)} + \left[\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)c_a + D\nabla_\Gamma^{\left(d_f\right)}c\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right] M^{\left(d_f;\delta d_f\right)} \,\mathrm{d}\Sigma \\
& + \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\left(\tau_{PG,\Gamma}^{\left(d_f;\delta d_f\right)} + \tau_{PG,\Gamma}^{\left(d_f;\delta\mathbf{u}\right)}\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right)M^{\left(d_f\right)} \\
& + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\delta\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c + \mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}c + \mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\delta c\right)\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right)M^{\left(d_f\right)} \\
& + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right)\left(\delta\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a + \mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}c_a\right)M^{\left(d_f\right)} + \tau_{PG,\Gamma}^{\left(d_f\right)}\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c\right) \\
& \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}c_a\right)M^{\left(d_f;\delta d_f\right)} \,\mathrm{d}\Sigma + \int_\Sigma f_{id,\Gamma}\bigg[r_f^2\nabla_\Gamma^{\left(d_f\right)}\delta\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \delta\gamma_f\gamma_{fa} - \delta\gamma\gamma_{fa} \\
& + r_f^2\left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \nabla_\Gamma^{\left(d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\gamma_{fa}\right)\bigg]M^{\left(d_f\right)} + f_{id,\Gamma}\bigg(r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_f \\
& \cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\bigg)M^{\left(d_f;\delta d_f\right)} + r_m^2\nabla_\Sigma\delta d_f\cdot\nabla_\Sigma d_{fa} + \delta d_f d_{fa} - A_d\delta d_m d_{fa}\,\mathrm{d}\Sigma
\end{aligned}
\tag{S-101}
$$

with the satisfication of the constraints in Eq. S-100 and

$$
\left.\begin{aligned}
& \delta\mathbf{u}\in\left(\mathcal{H}\left(\Sigma\right)\right)^3 \\
& \delta p\in\mathcal{H}\left(\Sigma\right) \\
& \delta\lambda\in\mathcal{L}^2\left(\Sigma\right) \\
& \delta c\in\mathcal{H}\left(\Sigma\right) \\
& \delta\gamma_f\in\mathcal{H}\left(\Sigma_D\right) \\
& \delta\gamma\in\mathcal{L}^2\left(\Sigma_D\right) \\
& \delta d_f\in\mathcal{H}\left(\Sigma\right) \\
& \delta d_m\in\mathcal{L}^2\left(\Sigma\right)
\end{aligned}\right\}
\text{ with }
\begin{cases}
\delta\mathbf{u} = \mathbf{0} \text{ at } \forall\mathbf{x}_\Sigma\in l_{v,\Sigma}\cup l_{v_0,\Sigma} \\
\delta\lambda = 0 \text{ at } \forall\mathbf{x}_\Sigma\in l_{v,\Sigma}\cup l_{v_0,\Sigma} \\
\delta c = 0 \text{ at } \forall\mathbf{x}_\Sigma\in l_{v,\Sigma}
\end{cases},
\tag{S-102}
$$

where δ is the first-order variational operator.

According to the Karush-Kuhn-Tucker conditions of the PDE constrained optimization problem [4], the first order variational of the augmented Lagrangian to c can be set to be zero as

$$
\begin{split}
& \int_{l_{s,\Sigma}} 2\left(c-\bar{c}\right) L^{\left(d_f\right)} \delta c \,\mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} \left(c_0-\bar{c}\right)^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\
& + \int_{\Sigma} \left[\left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \delta c \right) c_a + D \nabla_\Gamma^{\left(d_f\right)} \delta c \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma \\
& + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \delta c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0,
\end{split}
\tag{S-103}
$$

the first order variational of the augmented Lagrangian to $\mathbf{u}$, p and λ can be set to be zero as

$$
\begin{split}
& \int_{\Sigma} \left[\rho \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \right) \mathbf{u} \cdot \mathbf{u}_a + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \right) \delta\mathbf{u} \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \delta\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \delta\mathbf{u}^\mathrm{T} \right) \right. \\
& : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T} \right) - \delta p \,\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{\left(d_f\right)} \delta\mathbf{u} + \alpha \delta\mathbf{u} \cdot \mathbf{u}_a \\
& \left. + \left(\delta\lambda \mathbf{u}_a + \lambda_a \delta\mathbf{u} \right) \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) c_a \right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma \\
& + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left[- \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} \delta p \cdot \nabla_\Gamma^{\left(d_f\right)} p_a + \tau_{PG,\Gamma}^{\left(d_f;\delta\mathbf{u}\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) \right. \\
& + \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) + \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \\
& \left. \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) \right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0,
\end{split}
\tag{S-104}
$$

the first order variational of the augmented Lagrangian to γ_f can be set to be zero as

$$
\int_{\Sigma_D} \left(\frac{\partial\alpha}{\partial\gamma_p} \frac{\partial\gamma_p}{\partial\gamma_f} \mathbf{u} \cdot \mathbf{u}_a \delta\gamma_f + r_f^2 \nabla_\Gamma^{\left(d_f\right)} \delta\gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \delta\gamma_f \gamma_{fa} \right) M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0,
\tag{S-105}
$$

and the first order variational of the augmented Lagrangian to d_f can be set to be zero as

$$
\begin{aligned}
& \int_{l_{s,\Sigma}} (c-\bar{c})^2 L^{\left(d_f;\delta d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \int_{l_{v,\Sigma}} (c_0-\bar{c})^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} (c-\bar{c})^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\
& \int_{l_{v,\Sigma}} (c_0-\bar{c})^2 L^{\left(d_f;\delta d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \Big/ \left(\int_{l_{v,\Sigma}} (c_0-\bar{c})^2 L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \right)^2 + \int_\Sigma \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} \right) \mathbf{u} \right. \\
& \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f;\delta d_f\right)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T} \right) \\
& + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\delta d_f\right)} \mathbf{u}_a^\mathrm{T} \right) - p \,\mathrm{div}_\Gamma^{\left(d_f;\delta d_f\right)} \mathbf{u}_a \\
& \left. - p_a \mathrm{div}_\Gamma^{\left(d_f;\delta d_f\right)} \mathbf{u} + \left(\lambda \mathbf{u}_a + \lambda_a \mathbf{u}\right) \cdot \mathbf{n}_\Gamma^{\left(d_f;\delta d_f\right)} \right] M^{\left(d_f\right)} + \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \right) \mathbf{u} \cdot \mathbf{u}_a \right. \\
& + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T} \right) - p \,\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a \\
& \left. - p_a \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} \right] M^{\left(d_f;\delta d_f\right)} \\
& + \left[\left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} c \right) c_a + D \nabla_\Gamma^{\left(d_f;\delta d_f\right)} c \cdot \nabla_\Gamma^{\left(d_f\right)} c_a + D \nabla_\Gamma^{\left(d_f\right)} c \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} c_a \right] M^{\left(d_f\right)} \\
& + \left[\left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) c_a + D \nabla_\Gamma^{\left(d_f\right)} c \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right] M^{\left(d_f;\delta d_f\right)} \\
& + f_{id,\Gamma} r_f^2 \left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \nabla_\Gamma^{\left(d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} \gamma_{fa} \right) M^{\left(d_f\right)} \\
& + f_{id,\Gamma} \left(r_f^2 \nabla_\Gamma^{\left(d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa} \right) M^{\left(d_f;\delta d_f\right)} \\
& + r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa} \,\mathrm{d}\Sigma + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} - \tau_{BP,\Gamma}^{\left(d_f;\delta d_f\right)} \nabla_\Gamma^{\left(d_f\right)} p \cdot \nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)} \\
& - \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f;\delta d_f\right)} p \cdot \nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)} - \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} p \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} p_a M^{\left(d_f\right)} \\
& - \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} p \cdot \nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f;\delta d_f\right)} + \tau_{PG,\Gamma}^{\left(d_f;\delta d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) M^{\left(d_f\right)} \\
& + \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) M^{\left(d_f\right)} + \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \\
& \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\delta d_f\right)} c_a \right) M^{\left(d_f\right)} + \tau_{PG,\Gamma}^{\left(d_f\right)} \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} c_a \right) M^{\left(d_f;\delta d_f\right)} \,\mathrm{d}\Sigma = 0.
\end{aligned}
\tag{S-106}
$$

The constraints in Eqs. S-100 and S-102 are imposed to Eqs. S-103, S-104, S-105 and S-106. Then, the adjoint sensitivity of J_c is derived as

$$
\delta \hat{J}_c = - \int_{\Sigma_D} \gamma_{fa} \delta \gamma M^{\left(d_f\right)} \,\mathrm{d}\Sigma - \int_\Sigma A_d d_{fa} \delta d_m \,\mathrm{d}\Sigma. \tag{S-107}
$$

Without losing the arbitrariness of $\delta\mathbf{u}$, δp, $\delta\lambda$, δc, $\delta\gamma_f$, δd_f, $\delta\gamma$ and δd_m, one can set

$$
\left.
\begin{aligned}
& \tilde{\mathbf{u}}_a = \delta \mathbf{u} \\
& \tilde{p}_a = \delta p \\
& \tilde{\lambda}_a = \delta \lambda \\
& \tilde{c}_a = \delta c \\
& \tilde{\gamma}_{fa} = \delta \gamma_f \\
& \tilde{d}_{fa} = \delta d_f \\
& \tilde{\gamma} = \delta \gamma \\
& \tilde{d}_m = \delta d_m
\end{aligned}
\right\} \text{ with }
\left\{
\begin{aligned}
& \forall \tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\
& \forall \tilde{p}_a \in \mathcal{H}\left(\Sigma\right) \\
& \forall \tilde{\lambda}_a \in \mathcal{L}^2\left(\Sigma\right) \\
& \forall \tilde{c}_a \in \mathcal{H}\left(\Sigma\right) \\
& \forall \tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right) \\
& \forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right) \\
& \forall \tilde{\gamma} \in \mathcal{L}^2\left(\Sigma_D\right) \\
& \forall \tilde{d}_m \in \mathcal{L}^2\left(\Sigma\right)
\end{aligned}
\right.
\tag{S-108}
$$

for Eqs. S-103, S-104, S-105 and S-106 to derive the adjoint system composed of Eqs. S-90, S-91, S-93 and S-94.

S-6.9 Variational formulations of adjoint equations for pressure drop in Eq. 23

In Eq. 26, the adjoint variables γ_{fa} and d_{fa} are derived by sequentially solving the variational formulation for the adjoint equations of the surface Navier-Stokes equations

$$\left\{\begin{aligned}
&\text{Find}\left\{\begin{aligned}&\mathbf{u}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \text{ with } \mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma}\\ &p_a \in \mathcal{H}\left(\Sigma\right)\\ &\lambda_a \in \mathcal{L}^2\left(\Sigma\right) \text{ with } \lambda_a = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma}\end{aligned}\right.\\
&\text{for}\left\{\begin{aligned}&\forall \tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3\\ &\forall \tilde{p}_a \in \mathcal{H}\left(\Sigma\right)\\ &\forall \tilde{\lambda}_a \in \mathcal{L}^2\left(\Sigma\right)\end{aligned}\right., \text{ such that}\\
&\int_{l_{v,\Sigma}} \tilde{p}_a L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} \tilde{p}_a L^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} + \int_\Sigma \left[\rho \left(\tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{\left(d_f\right)}\right) \mathbf{u} \cdot \mathbf{u}_a + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)}\right) \tilde{\mathbf{u}}_a \right.\\
&\cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \tilde{\mathbf{u}}_a + \nabla_\Gamma^{\left(d_f\right)} \tilde{\mathbf{u}}_a^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T}\right) - \tilde{p}_a \,\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a\\
&\left. - p_a \mathrm{div}_\Gamma^{\left(d_f\right)} \tilde{\mathbf{u}}_a + \alpha \tilde{\mathbf{u}}_a \cdot \mathbf{u}_a + \tilde{\lambda}_a \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a \tilde{\mathbf{u}}_a \cdot \mathbf{n}_\Gamma^{\left(d_f\right)}\right] M^{\left(d_f\right)} \,\mathrm{d}\Sigma\\
&- \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} \tilde{p}_a \cdot \nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0
\end{aligned}\right. \tag{S-109}$$

and the variational formulations for the adjoint equations of the surface-PDE filters

$$\left\{\begin{aligned}
&\text{Find } \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \text{ for } \forall \tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right), \text{ such that}\\
&\int_{\Sigma_D} \left(\frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \mathbf{u}_a \tilde{\gamma}_{fa} + r_f^2 \nabla_\Gamma^{\left(d_f\right)} \tilde{\gamma}_{fa} \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \tilde{\gamma}_{fa} \gamma_{fa}\right) M^{\left(d_f\right)} \,\mathrm{d}\Sigma = 0
\end{aligned}\right. \tag{S-110}$$

and

$$\left\{\begin{aligned}
&\text{Find } d_{fa} \in \mathcal{H}\left(\Sigma\right) \text{ for } \forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right), \text{ such that}\\
&\int_{l_{v,\Sigma}} p L^{\left(d_f;\tilde{d}_{fa}\right)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} p L^{\left(d_f;\tilde{d}_{fa}\right)} \,\mathrm{d}l_{\partial\Sigma} + \int_\Sigma \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)}\right) \mathbf{u} \cdot \mathbf{u}_a \right.\\
&+ \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T}\right) + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} \right.\\
&\left. + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a^\mathrm{T}\right) - p \,\mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}\\
&+ \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} + f_{id,\Gamma} r_f^2 \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \nabla_\Gamma^{\left(d_f\right)} \gamma_f \right.\\
&\left.\left. \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \gamma_{fa}\right)\right] M^{\left(d_f\right)} + \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)}\right) \mathbf{u} \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a \right.\right.\\
&\left. + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^\mathrm{T}\right) - p \,\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{\left(d_f\right)}\\
&\left. + f_{id,\Gamma} \left(r_f^2 \nabla_\Gamma^{\left(d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa}\right)\right] M^{\left(d_f;\tilde{d}_{fa}\right)} + r_m^2 \nabla_\Sigma \tilde{d}_{fa} \cdot \nabla_\Sigma d_{fa}\\
&+ \tilde{d}_{fa} d_{fa} \,\mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left(\tau_{BP,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} \nabla_\Gamma^{\left(d_f\right)} p \cdot \nabla_\Gamma^{\left(d_f\right)} p_a + \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} p \right.\\
&\left. \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} p_a\right) M^{\left(d_f\right)} + \tau_{BP,\Gamma}^{\left(d_f\right)} \nabla_\Gamma^{\left(d_f\right)} p \cdot \nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f;\tilde{d}_{fa}\right)} \,\mathrm{d}\Sigma = 0.
\end{aligned}\right. \tag{S-111}$$

S-6.10 Adjoint analysis for constraint of pressure drop in Eq. 24

Based on the variational formulations of the surface Navier-Stokes equations in Eq. S-82 and the surface-PDE filters in Eqs. S-73 and S-74, the augmented Lagrangian of the pressure drop

ΔP in Eq. S-89 can be derived as

$$\begin{split}\widehat{\Delta P} = & \int_{l_{v,\Sigma}} pL^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} pL^{\left(d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\ & + \int_\Sigma \left[\rho \left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right)\right. \\ & - p\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u} + \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} \\ & \left. + f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right)\right] M^{\left(d_f\right)} \\ & + r_m^2\nabla_\Sigma d_f\cdot\nabla_\Sigma d_{fa} + d_f d_{fa} - A_d\left(d_m - \frac{1}{2}\right) d_{fa}\,\mathrm{d}\Sigma \\ & - \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma} \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)} p\cdot\nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)}\,\mathrm{d}\Sigma,\end{split} \tag{S-112}$$

where $\widehat{\Delta P}$ is the augmented lagrangian of ΔP; and the adjoint variables satisfy

$$\left.\begin{array}{l}\mathbf{u}_a\in\left(\mathcal{H}\left(\Sigma\right)\right)^3 \\ p_a\in\mathcal{H}\left(\Sigma\right) \\ \lambda_a\in\mathcal{L}^2\left(\Sigma\right) \\ \gamma_{fa}\in\mathcal{H}\left(\Sigma_D\right) \\ d_{fa}\in\mathcal{H}\left(\Sigma\right)\end{array}\right\} \text{ with } \begin{cases}\mathbf{u}_a = \mathbf{0} \text{ at } \forall\mathbf{x}_\Sigma\in l_{v,\Sigma}\cup l_{v_0,\Sigma} \\ \lambda_a = 0 \text{ at } \forall\mathbf{x}_\Sigma\in l_{v,\Sigma}\cup l_{v_0,\Sigma}\end{cases}. \tag{S-113}$$

Based on the related results in Section 2, the first order variational of $\widehat{\Delta P}$ can be derived as

$$\begin{split}\delta\widehat{\Delta P} = & \int_{l_{v,\Sigma}} \delta pL^{\left(d_f\right)} + pL^{\left(d_f;\delta d_f\right)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} \delta pL^{\left(d_f\right)} + pL^{\left(d_f;\delta d_f\right)} \,\mathrm{d}l_{\partial\Sigma} \\ & + \int_\Sigma \left[\rho\left(\delta\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\delta\mathbf{u}\cdot\mathbf{u}_a\right. \\ & + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\delta\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\delta\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) \\ & + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) \\ & + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}_a^\mathrm{T}\right) - \delta p\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a \\ & - p\,\mathrm{div}_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{\left(d_f;\delta d_f\right)}\mathbf{u} - p_a\mathrm{div}_\Gamma^{\left(d_f\right)}\delta\mathbf{u} + \alpha\delta\mathbf{u}\cdot\mathbf{u}_a + \frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u} \\ & \cdot\mathbf{u}_a\delta\gamma_f + \delta\lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f;\delta d_f\right)} + \lambda_a\delta\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f;\delta d_f\right)} \\ & + f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{\left(d_f\right)}\delta\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + r_f^2\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_f\right. \\ & \left.\left.\cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)}\gamma_{fa} + \delta\gamma_f\gamma_{fa} - \delta\gamma\gamma_{fa}\right)\right] M^{\left(d_f\right)} + \left[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a\right. \\ & + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a \\ & - p_a\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u} + \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} \\ & \left. + f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right)\right] M^{\left(d_f;\delta d_f\right)} + r_m^2\nabla_\Sigma\delta d_f \\ & \cdot\nabla_\Sigma d_{fa} + \delta d_f d_{fa} - A_d\delta d_m d_{fa}\,\mathrm{d}\Sigma - \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma} \tau_{BP,\Gamma}^{\left(d_f;\delta d_f\right)}\nabla_\Gamma^{\left(d_f\right)} p \\ & \cdot\nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)} + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)}\delta p\cdot\nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f\right)} + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)} p \\ & \cdot\nabla_\Gamma^{\left(d_f;\delta d_f\right)} p_a M^{\left(d_f\right)} + \tau_{BP,\Gamma}^{\left(d_f\right)}\nabla_\Gamma^{\left(d_f\right)} p\cdot\nabla_\Gamma^{\left(d_f\right)} p_a M^{\left(d_f;\delta d_f\right)}\,\mathrm{d}\Sigma\end{split} \tag{S-114}$$

with the satisfication of the constraints in Eq. S-113 and

$$\left.\begin{array}{l}\delta \mathbf{u} \in (\mathcal{H}(\Sigma))^3 \\ \delta p \in \mathcal{H}(\Sigma) \\ \delta \lambda \in \mathcal{L}^2(\Sigma) \\ \delta \gamma_f \in \mathcal{H}(\Sigma_D) \\ \delta \gamma \in \mathcal{L}^2(\Sigma_D) \\ \delta d_f \in \mathcal{H}(\Sigma) \\ \delta d_m \in \mathcal{L}^2(\Sigma)\end{array}\right\} \text{ with } \begin{cases}\delta \mathbf{u} = \mathbf{0} \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\ \delta \lambda = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma}\end{cases}. \tag{S-115}$$

According to the Karush-Kuhn-Tucker conditions of the PDE constrained optimization problem, the first order variational of the augmented Lagrangian to $\mathbf{u}$, p and λ can be set to be zero as

$$\begin{split}&\int_{l_{v,\Sigma}} \delta p L^{(d_f)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} \delta p L^{(d_f)} \,\mathrm{d}l_{\partial\Sigma} \\ &+ \int_\Sigma \left[\rho \left(\delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)}\right) \mathbf{u} \cdot \mathbf{u}_a + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)}\right) \delta \mathbf{u} \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \delta \mathbf{u} + \nabla_\Gamma^{(d_f)} \delta \mathbf{u}^\mathrm{T}\right)\right. \\ &: \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T}\right) - \delta p \,\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \delta \mathbf{u} + \alpha \delta \mathbf{u} \cdot \mathbf{u}_a + \delta \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} \\ &\left. + \lambda_a \delta \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)}\right] M^{(d_f)} \,\mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{BP,\Gamma}^{(d_f)} \nabla_\Gamma^{(d_f)} \delta p \cdot \nabla_\Gamma^{(d_f)} p_a M^{(d_f)} \,\mathrm{d}\Sigma = 0,\end{split} \tag{S-116}$$

the first order variational of the augmented Lagrangian to the variable γ_f can be set to be zero as

$$\int_{\Sigma_D} \left(\frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \mathbf{u}_a \delta \gamma_f + r_f^2 \nabla_\Gamma^{(d_f)} \delta \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \delta \gamma_f \gamma_{fa}\right) M^{(d_f)} \,\mathrm{d}\Sigma = 0, \tag{S-117}$$

and the first order variational of the augmented Lagrangian to the variable d_f can be set to be zero as

$$\begin{split}&\int_{l_{v,\Sigma}} p L^{(d_f;\delta d_f)} \,\mathrm{d}l_{\partial\Sigma} - \int_{l_{s,\Sigma}} p L^{(d_f;\delta d_f)} \,\mathrm{d}l_{\partial\Sigma} + \int_\Sigma \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)}\right) \mathbf{u} \cdot \mathbf{u}_a\right. \\ &+ \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T}\right) + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T}\right) \\ &: \left(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a^\mathrm{T}\right) - p \,\mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f;\delta d_f)} \\ &\left. + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f;\delta d_f)} + f_{id,\Gamma} \left(r_f^2 \nabla_\Gamma^{(d_f;\delta d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + r_f^2 \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \gamma_{fa}\right)\right] \\ &M^{(d_f)} + \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)}\right) \mathbf{u} \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T}\right)\right. \\ &- p \,\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} \\ &\left. + f_{id,\Gamma} \left(r_f^2 \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa}\right)\right] M^{(d_f;\delta d_f)} + r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} \\ &+ \delta d_f d_{fa} \,\mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{BP,\Gamma}^{(d_f;\delta d_f)} \nabla_\Gamma^{(d_f)} p \cdot \nabla_\Gamma^{(d_f)} p_a M^{(d_f)} + \tau_{BP,\Gamma}^{(d_f)} \nabla_\Gamma^{(d_f)} p \\ &\cdot \nabla_\Gamma^{(d_f;\delta d_f)} p_a M^{(d_f)} + \tau_{BP,\Gamma}^{(d_f)} \nabla_\Gamma^{(d_f)} p \cdot \nabla_\Gamma^{(d_f)} p_a M^{(d_f;\delta d_f)} \,\mathrm{d}\Sigma = 0.\end{split} \tag{S-118}$$

The constraints in Eqs. S-113 and S-115 are imposed to Eqs. S-116, S-117 and S-118. Then, the adjoint sensitivity of ΔP is derived as

$$\delta \widehat{\Delta P} = -\int_{\Sigma_D} \delta \gamma \gamma_{fa} M^{(d_f)} \,\mathrm{d}\Sigma - \int_\Sigma A_d \delta d_m d_{fa} \,\mathrm{d}\Sigma. \tag{S-119}$$

Without losing the arbitrariness of $\delta\mathbf{u}$, δp, $\delta\lambda$, $\delta\gamma_f$, δd_f, $\delta\gamma$ and δd_m, one can set

$$\left.\begin{aligned}
&\tilde{\mathbf{u}}_a = \delta\mathbf{u}\\
&\tilde{p}_a = \delta p\\
&\tilde{\lambda}_a = \delta\lambda\\
&\tilde{\gamma}_{fa} = \delta\gamma_f\\
&\tilde{d}_{fa} = \delta d_f\\
&\tilde{\gamma} = \delta\gamma\\
&\tilde{d}_m = \delta d_m
\end{aligned}\right\} \text{ with } \begin{cases}
\forall\tilde{\mathbf{u}}_a \in (\mathcal{H}(\Sigma))^3\\
\forall\tilde{p}_a \in \mathcal{H}(\Sigma)\\
\forall\tilde{\lambda}_a \in \mathcal{L}^2(\Sigma)\\
\forall\tilde{\gamma}_{fa} \in \mathcal{H}(\Sigma_D)\\
\forall\tilde{d}_{fa} \in \mathcal{H}(\Sigma)\\
\forall\tilde{\gamma} \in \mathcal{L}^2(\Sigma_D)\\
\forall\tilde{d}_m \in \mathcal{L}^2(\Sigma)
\end{cases} \tag{S-120}$$

for Eqs. S-116, S-117 and S-118 to derive the adjoint system composed of Eqs. S-109, S-110 and S-111.

S-6.11 Variational formulation of surface Navier-Stokes equations

For heat transfer, different stabilization term is chosen in the variational formulation of the surface Navier-Stokes equations to numerically solve the fluid velocity and pressure by using linear finite elements. The variational formulation of the surface Navier-Stokes equations can be derived as

$$\begin{cases}
\text{Find} \begin{cases}
\mathbf{u} \in (\mathcal{H}(\Gamma))^3 \text{ with } \begin{cases}\mathbf{u} = \mathbf{u}_{l_v,\Gamma} \text{ at } \forall\mathbf{x}_\Gamma \in l_{v,\Gamma}\\ \mathbf{u} = \mathbf{0} \text{ at } \forall\mathbf{x}_\Gamma \in l_{v_0,\Gamma}\end{cases}\\
p \in \mathcal{H}(\Gamma)\\
\lambda \in \mathcal{L}^2(\Gamma) \text{ with } \lambda = 0 \text{ at } \forall\mathbf{x}_\Gamma \in l_{v,\Gamma} \cup l_{v_0,\Gamma}
\end{cases}\\
\text{for} \begin{cases}
\forall\tilde{\mathbf{u}} \in (\mathcal{H}(\Gamma))^3\\
\forall\tilde{p} \in \mathcal{H}(\Gamma)\\
\forall\tilde{\lambda} \in \mathcal{L}^2(\Gamma)
\end{cases}, \text{ such that}\\
\int_\Gamma \rho(\mathbf{u}\cdot\nabla_\Gamma)\mathbf{u}\cdot\tilde{\mathbf{u}} + \frac{\eta}{2}\left(\nabla_\Gamma\mathbf{u} + \nabla_\Gamma\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma\tilde{\mathbf{u}} + \nabla_\Gamma\tilde{\mathbf{u}}^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma\tilde{\mathbf{u}} - \tilde{p}\,\mathrm{div}_\Gamma\mathbf{u}\\
+ \alpha\mathbf{u}\cdot\tilde{\mathbf{u}} + \lambda\tilde{\mathbf{u}}\cdot\mathbf{n}_\Gamma + \tilde{\lambda}\mathbf{u}\cdot\mathbf{n}_\Gamma \,\mathrm{d}\Gamma - \sum_{E_\Gamma\in\mathcal{E}_\Gamma}\int_{E_\Gamma} \tau_{LS\mathbf{u},\Gamma}\left(\rho\mathbf{u}\cdot\nabla_\Gamma\mathbf{u} + \nabla_\Gamma p + \alpha\mathbf{u}\right)\\
\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma\tilde{\mathbf{u}} + \nabla_\Gamma\tilde{p}\right) + \tau_{LSp,\Gamma}\left(\rho\mathrm{div}_\Gamma\mathbf{u}\right)\left(\mathrm{div}_\Gamma\tilde{\mathbf{u}}\right)\,\mathrm{d}\Gamma = 0
\end{cases} \tag{S-121}$$

where the general least square stabilization term is imposed as

$$-\sum_{E_\Gamma\in\mathcal{E}_\Gamma}\int_{E_\Gamma} \tau_{LS\mathbf{u},\Gamma}\left(\rho\mathbf{u}\cdot\nabla_\Gamma\mathbf{u} + \nabla_\Gamma p + \alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma\tilde{\mathbf{u}} + \nabla_\Gamma\tilde{p}\right) + \tau_{LSp,\Gamma}\left(\rho\mathrm{div}_\Gamma\mathbf{u}\right)\left(\mathrm{div}_\Gamma\tilde{\mathbf{u}}\right)\,\mathrm{d}\Gamma \tag{S-122}$$

with $\tau_{LS\mathbf{u},\Gamma}$ and $\tau_{LSp,\Gamma}$ representing the stabilization parameters. The stabilization parameters are set as [3]

$$\begin{cases}
\tau_{LS\mathbf{u},\Gamma} = \min\left(\frac{h_{E_\Gamma}}{2\rho\left\|\mathbf{u}\right\|_2}, \frac{h_{E_\Gamma}^2}{12\eta}\right)\\
\tau_{LSp,\Gamma} = \begin{cases}\frac{1}{2}h_{E_\Gamma}\left\|\mathbf{u}\right\|_2, \ \mathbf{u}^2 < \epsilon_{eps}^{\frac{1}{2}}\\ \frac{1}{2}h_{E_\Gamma}, \ \mathbf{u}^2 \geq \epsilon_{eps}^{\frac{1}{2}}\end{cases}
\end{cases} \tag{S-123}$$

where ϵ_{eps} with the value of 2.2×10^{-16} is the floating point precision. Based on Eqs. S-69, S-79 and S-80, the stabilization parameters in Eq. S-123 can be transformed into

$$\begin{cases}
\tau_{LS\mathbf{u},\Gamma}^{(d_f)} = \min\left(\frac{h_{E_\Sigma}}{2\rho\left\|\mathbf{u}\right\|_2}\left(M^{(d_f)}\right)^{\frac{1}{2}}, \frac{h_{E_\Sigma}^2}{12\eta}M^{(d_f)}\right)\\
\tau_{LSp,\Gamma}^{(d_f)} = \begin{cases}\frac{1}{2}h_{E_\Sigma}\left\|\mathbf{u}\right\|_2\left(M^{(d_f)}\right)^{\frac{1}{2}}, \ \mathbf{u}^2 < \epsilon_{eps}^{\frac{1}{2}}\\ \frac{1}{2}h_{E_\Sigma}\left(M^{(d_f)}\right)^{\frac{1}{2}}, \ \mathbf{u}^2 \geq \epsilon_{eps}^{\frac{1}{2}}\end{cases}
\end{cases}. \tag{S-124}$$

Based on the coupling relations in Section 2.2.3, the variational formulation in Eq. S-121 can be transformed into the form defined on the base manifold Σ:

$$\begin{cases} \text{Find} \begin{cases} \mathbf{u} \in (\mathcal{H}(\Sigma))^3 \text{ with } \begin{cases} \mathbf{u} = \mathbf{u}_{l_v,\Sigma} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \\ \mathbf{u} = \mathbf{0} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v_0,\Sigma} \end{cases} \\ p \in \mathcal{H}(\Sigma) \\ \lambda \in \mathcal{L}^2(\Sigma) \text{ with } \lambda = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \end{cases} \\ \text{for} \begin{cases} \forall \tilde{\mathbf{u}} \in (\mathcal{H}(\Sigma))^3 \\ \forall \tilde{p} \in \mathcal{H}(\Sigma) \\ \forall \tilde{\lambda} \in \mathcal{L}^2(\Sigma) \end{cases}, \text{ such that} \\ \int_\Sigma \left[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \mathbf{u} \cdot \tilde{\mathbf{u}} + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}} + \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}^\mathrm{T} \right) \right. \\ \left. - p \,\mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}} - \tilde{p} \,\mathrm{div}_\Gamma^{(d_f)} \mathbf{u} + \alpha \mathbf{u} \cdot \tilde{\mathbf{u}} + \lambda \tilde{\mathbf{u}} \cdot \mathbf{n}_\Gamma^{(d_f)} + \tilde{\lambda} \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} \right] M^{(d_f)} \,\mathrm{d}\Sigma \\ - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left[\tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}} \right.\right. \\ \left.\left. + \nabla_\Gamma^{(d_f)} \tilde{p} \right) + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}} \right) \right] M^{(d_f)} \,\mathrm{d}\Sigma = 0. \end{cases} \tag{S-125}$$

S-6.12 Variational formulation of the surface convective heat-transfer equation

Based on the Galerkin method, the variational formulation of the surface convective heat-transfer equation is considered in the first order Sobolev space defined on the implicit 2-manifold Γ:

$$\begin{cases} \text{Find } T \in \mathcal{H}(\Gamma) \text{ with } T = T_0 \text{ at } \forall \mathbf{x}_\Gamma \in l_{v,\Gamma}, \text{ for } \forall \tilde{T} \in \mathcal{H}(\Gamma), \\ \text{such that } \int_\Gamma (\rho C_p \mathbf{u} \cdot \nabla_\Gamma T - Q) \tilde{T} + k \nabla_\Gamma T \cdot \nabla_\Gamma \tilde{T} \,\mathrm{d}\Gamma \\ + \sum_{E_\Gamma \in \mathcal{E}_\Gamma} \int_{E_\Gamma} \tau_{LST,\Gamma} (\rho C_p \mathbf{u} \cdot \nabla_\Gamma T - Q) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma \tilde{T} \right) \mathrm{d}\Gamma = 0 \end{cases} \tag{S-126}$$

where $\tilde{T}$ is the test function of T; and the general least square stabilization term

$$\sum_{E_\Gamma \in \mathcal{E}_\Gamma} \int_{E_\Gamma} \tau_{LST,\Gamma} (\rho C_p \mathbf{u} \cdot \nabla_\Gamma T - Q) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma \tilde{T} \right) \mathrm{d}\Gamma \tag{S-127}$$

with $\tau_{LST,\Gamma}$ representing the stabilization parameter is imposed on the variational formulation, in order to use linear finite elements to solve Eq. 27 [3]. The stabilization parameter is expressed as [3]

$$\tau_{LST,\Gamma} = \min \left(\frac{h_{E_\Gamma}}{2\rho C_p \|\mathbf{u}\|_2}, \frac{h_{E_\Gamma}^2}{12k} \right). \tag{S-128}$$

Based on Eqs. S-69, S-79 and S-80, $\tau_{LST,\Gamma}$ can be transformed into

$$\tau_{LST,\Gamma}^{(d_f)} = \min \left(\frac{h_{E_\Sigma}}{2\rho C_p \|\mathbf{u}\|_2} \left(M^{(d_f)} \right)^{\frac{1}{2}}, \frac{h_{E_\Sigma}^2}{12k} M^{(d_f)} \right). \tag{S-129}$$

Based on the homeomorphisms and the coupling relations in Section 2.2.3, the variational formulation in Eq. S-83 can be transformed into the form defined on the base manifold Σ:

$$\begin{cases} \text{Find } c \in \mathcal{H}(\Sigma) \text{ with } c = c_0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma}, \text{ for } \forall \tilde{c} \in \mathcal{H}(\Sigma), \\ \text{such that } \int_\Sigma \left[\left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \tilde{T} + k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} \tilde{T} \right] M^{(d_f)} \,\mathrm{d}\Sigma \\ + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{T} \right) M^{(d_f)} \,\mathrm{d}\Sigma = 0. \end{cases} \tag{S-130}$$

S-6.13 Transformation of design objective in Eq. 30, dissipation power in Eq. 32 and area fraction in Eq. 34

Based on the coupling relations in Section 2.2.3, the design objective in Eq. 30 can be transformed into

$$J_T^{(d_f)} = \int_\Sigma f_{id,\Gamma} k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T M^{(d_f)} \,\mathrm{d}\Sigma. \tag{S-131}$$

Based on the coupling relations in Section 2.2.3, the dissipation power in Eq. 32 can be transformed into

$$\Phi^{(d_f)} = \int_\Sigma \left[\frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) + \alpha \mathbf{u}^2 \right] M^{(d_f)} \,\mathrm{d}\Sigma. \tag{S-132}$$

Based on the coupling relations in Section 2.2.3, the area fraction in Eq. 34 can be transformed into

$$s^{(d_f)} = \frac{1}{|\Gamma_D|^{(d_f)}} \int_{\Sigma_D} \gamma_p M^{(d_f)} \,\mathrm{d}\Sigma = \frac{1}{|\Gamma_D|^{(d_f)}} \int_\Sigma f_{id,\Gamma} \gamma_p M^{(d_f)} \,\mathrm{d}\Sigma \tag{S-133}$$

with

$$|\Gamma_D|^{(d_f)} = \int_{\Sigma_D} M^{(d_f)} \,\mathrm{d}\Sigma = \int_\Sigma f_{id,\Gamma} M^{(d_f)} \,\mathrm{d}\Sigma. \tag{S-134}$$

S-6.14 Variational formulations of adjoint equations for design objective in Eq. 30

The variational formulation for the adjoint equation of the surface convective heat-transfer equation is derived as

$$\left\{ \begin{aligned} & \text{Find } T_a \in \mathcal{H}(\Sigma) \text{ with } T_a = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma}, \text{ for } \forall \tilde{T}_a \in \mathcal{H}(\Sigma), \text{ such that} \\ & \int_\Sigma \left[2 f_{id,\Gamma} k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} \tilde{T}_a + \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{T}_a \right) T_a + k \nabla_\Gamma^{(d_f)} T_a \cdot \nabla_\Gamma^{(d_f)} \tilde{T}_a \right] \\ & M^{(d_f)} \,\mathrm{d}\Sigma + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{T}_a \right) M^{(d_f)} \,\mathrm{d}\Sigma = 0 \end{aligned} \right. \tag{S-135}$$

where T_a is the adjoint variable of T and $\tilde{T}_a$ is the test function of T_a. The variational formulation for the adjoint equations of the surface Naiver-Stokes equations is derived as

$$\left\{ \begin{aligned} & \text{Find} \left\{ \begin{aligned} & \mathbf{u}_a \in (\mathcal{H}(\Sigma))^3 \text{ with } \mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\ & p_a \in \mathcal{H}(\Sigma) \\ & \lambda_a \in \mathcal{L}^2(\Sigma) \text{ with } \lambda_a = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \end{aligned} \right. \\ & \text{for} \left\{ \begin{aligned} & \forall \tilde{\mathbf{u}}_a \in (\mathcal{H}(\Sigma))^3 \\ & \forall \tilde{p}_a \in \mathcal{H}(\Sigma) \\ & \forall \tilde{\lambda}_a \in \mathcal{L}^2(\Sigma) \end{aligned} \right. , \text{ such that} \\ & \int_\Sigma \left[\rho \left(\tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a \right) \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a + \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) \right. \\ & \left. - \tilde{p}_a \mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a + \alpha \tilde{\mathbf{u}}_a \cdot \mathbf{u}_a + \tilde{\lambda}_a \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \tilde{\mathbf{u}}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \rho C_p \tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} T T_a \right] \\ & M^{(d_f)} \,\mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left\{ \tau_{LS\mathbf{u},\Gamma}^{(d_f;\tilde{\mathbf{u}}_a)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \right. \\ & + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left[\rho \left(\tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a \right) + \nabla_\Gamma^{(d_f)} \tilde{p}_a + \alpha \tilde{\mathbf{u}}_a \right] \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \\ & + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f;\tilde{\mathbf{u}}_a)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \\ & \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) - \tau_{LST,\Gamma}^{(d_f;\tilde{\mathbf{u}}_a)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \\ & \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) - \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) - \tau_{LST,\Gamma}^{(d_f)} \\ & \left. \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\rho C_p \tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} T_a \right) \right\} M^{(d_f)} \,\mathrm{d}\Sigma = 0 \end{aligned} \right. \tag{S-136}$$

where $\tau_{LS\mathbf{u},\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)}$, $\tau_{LSp,\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)}$ and $\tau_{LST,\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)}$ are the first-order variationals of $\tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)}$, $\tau_{LSp,\Gamma}^{\left(d_f\right)}$ and $\tau_{LST,\Gamma}^{\left(d_f\right)}$ to $\mathbf{u}$, respectively, and they are expressed as

$$\left.\begin{aligned}
&\tau_{LS\mathbf{u},\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)} = \begin{cases} -\dfrac{h_{E_\Sigma}\mathbf{u}\cdot\tilde{\mathbf{u}}_a}{2\rho\left\|\mathbf{u}\right\|_2^3}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}, & \dfrac{h_{E_\Sigma}}{2\rho\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} < \dfrac{h_{E_\Sigma}^2}{12\eta}M^{\left(d_f\right)} \\ 0, & \dfrac{h_{E_\Sigma}}{2\rho\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} \geq \dfrac{h_{E_\Sigma}^2}{12\eta}M^{\left(d_f\right)} \end{cases} \\
&\tau_{LSp,\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)} = \begin{cases} \dfrac{h_{E_\Sigma}\mathbf{u}\cdot\tilde{\mathbf{u}}_a}{2\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}, & \mathbf{u}^2 < \epsilon_{eps}^{\frac{1}{2}} \\ 0, & \mathbf{u}^2 \geq \epsilon_{eps}^{\frac{1}{2}} \end{cases} \\
&\tau_{LST,\Gamma}^{\left(d_f;\tilde{\mathbf{u}}_a\right)} = \begin{cases} -\dfrac{h_{E_\Sigma}\mathbf{u}\cdot\tilde{\mathbf{u}}_a}{2\rho C_p\left\|\mathbf{u}\right\|_2^3}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}, & \dfrac{h_{E_\Sigma}}{2\rho C_p\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} < \dfrac{h_{E_\Sigma}^2}{12k}M^{\left(d_f\right)} \\ 0, & \dfrac{h_{E_\Sigma}}{2\rho C_p\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} \geq \dfrac{h_{E_\Sigma}^2}{12k}M^{\left(d_f\right)} \end{cases} \\
&\forall\tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3.
\end{aligned}\right\} \tag{S-137}$$

The variational formulations for the adjoint equations of the surface-PDE filters for γ and d_m are derived as

$$\begin{cases}
\text{Find } \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \text{ for } \forall\tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right), \text{ such that} \\
\displaystyle\int_{\Sigma_D}\left\{\left[\frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\mathbf{u}_a + \rho\frac{\partial C_p}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}TT_a + \frac{\partial k}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\left(f_{id,\Gamma}\nabla_\Gamma^{\left(d_f\right)}T\right.\right.\right. \\
\displaystyle\left.\left.\cdot\nabla_\Gamma^{\left(d_f\right)}T + \nabla_\Gamma^{\left(d_f\right)}T\cdot\nabla_\Gamma^{\left(d_f\right)}T_a\right)\right]\tilde{\gamma}_{fa} + r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa}\cdot\nabla_\Gamma^{\left(d_f\right)}\tilde{\gamma}_{fa} + \gamma_{fa}\tilde{\gamma}_{fa}\Big\}M^{\left(d_f\right)}\,\mathrm{d}\Sigma \\
\displaystyle-\sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma\cap\Sigma_D}\left\{\tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)}\frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}p_a\right) - \left(\frac{\partial\tau_{LST,\Gamma}^{\left(d_f\right)}}{\partial C_p}\frac{\partial C_p}{\partial\gamma_p}\right.\right. \\
\displaystyle\left.+\frac{\partial\tau_{LST,\Gamma}^{\left(d_f\right)}}{\partial k}\frac{\partial k}{\partial\gamma_p}\right)\frac{\partial\gamma_p}{\partial\gamma_f}\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T - Q\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T_a\right) - \tau_{LST,\Gamma}^{\left(d_f\right)}\rho\frac{\partial C_p}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f} \\
\displaystyle\left[\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T_a\right) + \left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T - Q\right)\right. \\
\displaystyle\left.\left.\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T_a\right)\right]\right\}\tilde{\gamma}_{fa}M^{\left(d_f\right)}\,\mathrm{d}\Sigma = 0
\end{cases} \tag{S-138}$$

and

$$\begin{cases}
\text{Find } d_{fa} \in \mathcal{H}(\Sigma) \ \text{ for } \forall \tilde{d}_{fa} \in \mathcal{H}(\Sigma), \ \text{ such that} \\
\displaystyle\int_\Sigma \left[2 f_{id,\Gamma} k \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} T \cdot \nabla_\Gamma^{\left(d_f\right)} T + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \right) \mathbf{u} \cdot \mathbf{u}_a \right. \\
+ \dfrac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}^{\mathrm{T}} \right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^{\mathrm{T}} \right) + \dfrac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^{\mathrm{T}} \right) \\
: \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a^{\mathrm{T}} \right) - p \, \mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u} + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} + \lambda_a \\
\mathbf{u} \cdot \mathbf{n}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} + \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} T \right) T_a + k \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} T \cdot \nabla_\Gamma^{\left(d_f\right)} T_a + k \nabla_\Gamma^{\left(d_f\right)} T \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} T_a \\
+ f_{id,\Gamma} r_f^2 \left(\nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \nabla_\Gamma^{\left(d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \gamma_{fa} \right) \Big] M^{\left(d_f\right)} + \Big[f_{id,\Gamma} k \nabla_\Gamma^{\left(d_f\right)} T \\
\cdot \nabla_\Gamma^{\left(d_f\right)} T + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \right) \mathbf{u} \cdot \mathbf{u}_a + \dfrac{\eta}{2} \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}^{\mathrm{T}} \right) : \left(\nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a^{\mathrm{T}} \right) \\
- p \, \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a - p_a \, \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{\left(d_f\right)} + \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T - Q \right) \\
T_a + k \nabla_\Gamma^{\left(d_f\right)} T \cdot \nabla_\Gamma^{\left(d_f\right)} T_a + f_{id,\Gamma} \left(r_f^2 \nabla_\Gamma^{\left(d_f\right)} \gamma_f \cdot \nabla_\Gamma^{\left(d_f\right)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa} \right) \Big] M^{\left(d_f;\tilde{d}_{fa}\right)} \\
+ r_m^2 \nabla_\Sigma \tilde{d}_{fa} \cdot \nabla_\Sigma d_{fa} + \tilde{d}_{fa} d_{fa} \, \mathrm{d}\Sigma - \displaystyle\sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left[\tau_{LS\mathbf{u},\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} p + \alpha \mathbf{u} \right) \right. \\
\cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} p_a \right) + \tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} p \right) \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a \right. \\
\left. + \nabla_\Gamma^{\left(d_f\right)} p_a \right) + \tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} p_a \right) \\
+ \tau_{LSp,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} \left(\rho \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{\left(d_f\right)} \left(\rho \mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{\left(d_f\right)} \\
\left(\rho \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} \mathbf{u}_a \right) - \tau_{LST,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T - Q \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T_a \right) \\
- \tau_{LST,\Gamma}^{\left(d_f\right)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T_a \right) - \tau_{LST,\Gamma}^{\left(d_f\right)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T - Q \right) \\
\left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f;\tilde{d}_{fa}\right)} T_a \right) \Big] M^{\left(d_f\right)} + \Big[\tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \mathbf{u} + \nabla_\Gamma^{\left(d_f\right)} p + \alpha \mathbf{u} \right) \\
\cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} \mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)} p_a \right) + \tau_{LSp,\Gamma}^{\left(d_f\right)} \left(\rho \mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{\left(d_f\right)} \mathbf{u}_a \right) - \tau_{LST,\Gamma}^{\left(d_f\right)} \\
\left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T - Q \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{\left(d_f\right)} T_a \right) \Big] M^{\left(d_f;\tilde{d}_{fa}\right)} \, \mathrm{d}\Sigma = 0
\end{cases} \tag{S-139}$$

where $\tau_{LS\mathbf{u},\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)}$, $\tau_{LSp,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)}$ and $\tau_{LST,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)}$ are the first-order variationals of $\tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)}$, $\tau_{LSp,\Gamma}^{\left(d_f\right)}$ and $\tau_{LST,\Gamma}^{\left(d_f\right)}$ to d_f, respectively, and they are derived as

$$\left.\begin{aligned}
&\tau_{LS\mathbf{u},\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} = \begin{cases} \dfrac{h_{E_\Sigma}}{4\rho\left\|\mathbf{u}\right\|_2\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}} M^{\left(d_f;\tilde{d}_{fa}\right)}, & \dfrac{h_{E_\Sigma}}{2\rho\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} < \dfrac{h_{E_\Sigma}^2}{12\eta} M^{\left(d_f\right)} \\ \dfrac{h_{E_\Sigma}^2}{12\eta} M^{\left(d_f;\tilde{d}_{fa}\right)}, & \dfrac{h_{E_\Sigma}}{2\rho\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} \geq \dfrac{h_{E_\Sigma}^2}{12\eta} M^{\left(d_f\right)} \end{cases} \\
&\tau_{LSp,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} = \begin{cases} \dfrac{h_{E_\Sigma}\left\|\mathbf{u}\right\|_2}{4\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}} M^{\left(d_f;\tilde{d}_{fa}\right)}, & \mathbf{u}^2 < \epsilon_{eps}^{\frac{1}{2}} \\ \dfrac{h_{E_\Sigma}}{4\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}} M^{\left(d_f;\tilde{d}_{fa}\right)}, & \mathbf{u}^2 \geq \epsilon_{eps}^{\frac{1}{2}} \end{cases} \\
&\tau_{LST,\Gamma}^{\left(d_f;\tilde{d}_{fa}\right)} = \begin{cases} \dfrac{h_{E_\Sigma}}{4\rho C_p\left\|\mathbf{u}\right\|_2\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}}} M^{\left(d_f;\tilde{d}_{fa}\right)}, & \dfrac{h_{E_\Sigma}}{2\rho C_p\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} < \dfrac{h_{E_\Sigma}^2}{12k} M^{\left(d_f\right)} \\ \dfrac{h_{E_\Sigma}^2}{12k} M^{\left(d_f;\tilde{d}_{fa}\right)}, & \dfrac{h_{E_\Sigma}}{2\rho C_p\left\|\mathbf{u}\right\|_2}\left(M^{\left(d_f\right)}\right)^{\frac{1}{2}} \geq \dfrac{h_{E_\Sigma}^2}{12k} M^{\left(d_f\right)} \end{cases}
\end{aligned}\right\}$$
$$\forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right). \tag{S-140}$$

S-6.15 Adjoint analysis for design objective in Eq. 36

Based on the transformed design objective in Eq. S-131, the variational formulations of the surface-PDE filters in Eqs. S-73 and S-74 and the surface Navier-Stokes equations in Eq. S-125 and the surface convective heat-transfer equation in Eq. S-130, the augmented Lagrangian of the design objective in Eq. 36 can be derived as

$$\begin{aligned}
\hat{J}_T = & \int_\Sigma f_{id,\Gamma} k \nabla_\Gamma^{\left(d_f\right)} T \cdot \nabla_\Gamma^{\left(d_f\right)} T M^{\left(d_f\right)} + \left[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\right)\mathbf{u}\cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}^\mathrm{T}\right)\right. \\
& : \left(\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a - p_a\,\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u} + \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{\left(d_f\right)} \\
& \left. + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{\left(d_f\right)}\right] M^{\left(d_f\right)}\,\mathrm{d}\Sigma - \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\tau_{LS\mathbf{u},\Gamma}^{\left(d_f\right)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\mathbf{u} + \nabla_\Gamma^{\left(d_f\right)}p + \alpha\mathbf{u}\right) \\
& \cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}\mathbf{u}_a + \nabla_\Gamma^{\left(d_f\right)}p_a\right) M^{\left(d_f\right)} + \tau_{LSp,\Gamma}^{\left(d_f\right)}\left(\rho\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{\left(d_f\right)}\mathbf{u}_a\right) M^{\left(d_f\right)}\,\mathrm{d}\Sigma \\
& + \int_\Sigma\left[\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T - Q\right)T_a + k\nabla_\Gamma^{\left(d_f\right)}T\cdot\nabla_\Gamma^{\left(d_f\right)}T_a\right] M^{\left(d_f\right)}\,\mathrm{d}\Sigma \\
& + \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\tau_{LST,\Gamma}^{\left(d_f\right)}\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T - Q\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{\left(d_f\right)}T_a\right) M^{\left(d_f\right)}\,\mathrm{d}\Sigma \\
& + \int_\Sigma f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{\left(d_f\right)}\gamma_f\cdot\nabla_\Gamma^{\left(d_f\right)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right) M^{\left(d_f\right)} \\
& + r_m^2\nabla_\Sigma d_f\cdot\nabla_\Sigma d_{fa} + d_f d_{fa} - A_d\left(d_m - \frac{1}{2}\right) d_{fa}\,\mathrm{d}\Sigma,
\end{aligned} \tag{S-141}$$

where $\hat{J}_T$ is the augmented lagrangian of J_T; and the adjoint variables satisfy

$$\left.\begin{aligned} & \mathbf{u}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\ & p_a \in \mathcal{H}\left(\Sigma\right) \\ & \lambda_a \in \mathcal{L}^2\left(\Sigma\right) \\ & T_a \in \mathcal{H}\left(\Sigma\right) \\ & \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \\ & d_{fa} \in \mathcal{H}\left(\Sigma\right) \end{aligned}\right\} \text{ with } \begin{cases} \mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x} \in l_{v,\Sigma}\cup l_{v_0,\Sigma} \\ \lambda_a = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma}\cup l_{v_0,\Sigma} \\ T_a = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \end{cases}. \tag{S-142}$$

The first order variational of the augmented Lagrangian in Eq. S-141 can be derived as

$$
\begin{aligned}
\delta \hat{J}_T = & \int_\Sigma f_{id,\Gamma} \frac{\partial k}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T M^{(d_f)} \delta\gamma_f + 2 f_{id,\Gamma} k \nabla_\Gamma^{(d_f;\delta d_f)} T \cdot \nabla_\Gamma^{(d_f)} T M^{(d_f)} \\
& + 2 f_{id,\Gamma} k \nabla_\Gamma^{(d_f)} \delta T \cdot \nabla_\Gamma^{(d_f)} T M^{(d_f)} + f_{id,\Gamma} k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T M^{(d_f;\delta d_f)} \\
& + \Big[\rho \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \mathbf{u} \cdot \mathbf{u}_a + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \right) \mathbf{u} \cdot \mathbf{u}_a + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \delta\mathbf{u} \cdot \mathbf{u}_a \\
& + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \delta\mathbf{u} + \nabla_\Gamma^{(d_f)} \delta\mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) \\
& + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) + \frac{\eta}{2} \Big(\nabla_\Gamma^{(d_f)} \mathbf{u} \\
& + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \Big) : \left(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a^\mathrm{T} \right) - \delta p \, \mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p \, \mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a \\
& - p_a \mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u} - p_a \mathrm{div}_\Gamma^{(d_f)} \delta\mathbf{u} + \frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \mathbf{u}_a \delta\gamma_f + \alpha \delta\mathbf{u} \cdot \mathbf{u}_a + \delta\lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} \\
& + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f;\delta d_f)} + \lambda_a \delta\mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f;\delta d_f)} \Big] M^{(d_f)} + \Big[\rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \mathbf{u} \cdot \mathbf{u}_a \\
& + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) - p \, \mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \\
& + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} \Big] M^{(d_f;\delta d_f)} \, \mathrm{d}\Sigma \\
& - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left(\tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta d_f)} + \tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta \mathbf{u})} \right) \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \Big(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a \\
& + \nabla_\Gamma^{(d_f)} p_a \Big) M^{(d_f)} + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \Big[\rho \Big(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta\mathbf{u} \Big) \\
& + \nabla_\Gamma^{(d_f;\delta d_f)} p + \nabla_\Gamma^{(d_f)} \delta p + \alpha \delta\mathbf{u} + \frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \delta\gamma_f \Big] \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) M^{(d_f)} \\
& + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \Big[\rho \Big(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a \Big) \\
& + \nabla_\Gamma^{(d_f;\delta d_f)} p_a \Big] M^{(d_f)} + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \Big(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a \\
& + \nabla_\Gamma^{(d_f)} p_a \Big) M^{(d_f;\delta d_f)} + \left(\tau_{LSp,\Gamma}^{(d_f;\delta d_f)} + \tau_{LSp,\Gamma}^{(d_f;\delta \mathbf{u})} \right) \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) M^{(d_f)} \\
& + \tau_{LSp,\Gamma}^{(d_f)} \rho \left(\mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \mathrm{div}_\Gamma^{(d_f)} \delta\mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) M^{(d_f)} + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \\
& \left(\mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a \right) M^{(d_f)} + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) M^{(d_f;\delta d_f)} \, \mathrm{d}\Sigma \\
& + \int_\Sigma \Big[\rho C_p \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} T + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta T \right) T_a + \rho \frac{\partial C_p}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T \\
& T_a \delta\gamma_f + \frac{\partial k}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T_a \delta\gamma_f + k \nabla_\Gamma^{(d_f;\delta d_f)} T \cdot \nabla_\Gamma^{(d_f)} T_a + k \nabla_\Gamma^{(d_f)} \delta T \cdot \nabla_\Gamma^{(d_f)} T_a \\
& + k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f;\delta d_f)} T_a \Big] M^{(d_f)} + \Big[\left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) T_a + k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T_a \Big] \\
& M^{(d_f;\delta d_f)} \, \mathrm{d}\Sigma + \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \left(\tau_{LST,\Gamma}^{(d_f;\delta d_f)} + \tau_{LST,\Gamma}^{(d_f;\delta \mathbf{u})} \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \\
& \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) M^{(d_f)}
\end{aligned}
\tag{S-143}
$$

$$
\begin{aligned}
&+ \tau_{LST,\Gamma}^{(d_f)} \rho C_p \left(\delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} T + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) M^{(d_f)} \\
&+ \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \rho C_p \left(\delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} T_a \right) M^{(d_f)} \\
&+ \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) M^{(d_f;\delta d_f)} + \left(\frac{\partial \tau_{LST,\Gamma}^{(d_f)}}{\partial C_p} \frac{\partial C_p}{\partial \gamma_p} \right. \\
&+ \left. \frac{\partial \tau_{LST,\Gamma}^{(d_f)}}{\partial k} \frac{\partial k}{\partial \gamma_p} \right) \frac{\partial \gamma_p}{\partial \gamma_f} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) M^{(d_f)} \delta \gamma_f \\
&+ \tau_{LST,\Gamma}^{(d_f)} \rho \frac{\partial C_p}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \Big[\left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) \\
&+ \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) \Big] M^{(d_f)} \delta \gamma_f \,\mathrm{d}\Sigma \\
&+ \int_\Sigma f_{id,\Gamma} \Big[r_f^2 \Big(\nabla_\Gamma^{(d_f)} \delta \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \nabla_\Gamma^{(d_f;\delta d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \gamma_{fa} \Big) \\
&+ \delta \gamma_f \gamma_{fa} - \delta \gamma \gamma_{fa} \Big] M^{(d_f)} + f_{id,\Gamma} \left(r_f^2 \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa} \right) M^{(d_f;\delta d_f)} \\
&+ r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa} - A_d \delta d_m d_{fa} \,\mathrm{d}\Sigma
\end{aligned}
$$

with the satisfication of the constraints in Eq. S-142 and

$$
\left.
\begin{aligned}
&\delta \mathbf{u} \in \left(\mathcal{H}(\Sigma) \right)^3 \\
&\delta p \in \mathcal{H}(\Sigma) \\
&\delta \lambda \in \mathcal{L}^2(\Sigma) \\
&\delta T \in \mathcal{H}(\Sigma) \\
&\delta \gamma_f \in \mathcal{H}(\Sigma_D) \\
&\delta \gamma \in \mathcal{L}^2(\Sigma_D) \\
&\delta d_f \in \mathcal{H}(\Sigma) \\
&\delta d_m \in \mathcal{L}^2(\Sigma)
\end{aligned}
\right\} \text{ with }
\begin{cases}
\delta \mathbf{u} = \mathbf{0} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\
\delta \lambda = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\
\delta T = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma}
\end{cases}. \tag{S-144}
$$

According to the Karush-Kuhn-Tucker conditions of the PDE constrained optimization problem [4], the first order variational of the augmented Lagrangian to T can be set to be zero as

$$
\begin{aligned}
&\int_\Sigma \left(2 f_{id,\Gamma} k \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} \delta T + \rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta T T_a + k \nabla_\Gamma^{(d_f)} \delta T \cdot \nabla_\Gamma^{(d_f)} T_a \right) M^{(d_f)} \,\mathrm{d}\Sigma \\
&+ \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) M^{(d_f)} \,\mathrm{d}\Sigma = 0,
\end{aligned} \tag{S-145}
$$

the first order variational of the augmented Lagrangian to $\mathbf{u}$, p and λ can be set to be zero as

$$
\begin{aligned}
&\int_\Sigma \Big[\rho \left(\delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta \mathbf{u} \right) \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \delta \mathbf{u} + \nabla_\Gamma^{(d_f)} \delta \mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) \\
&- \delta p \,\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \delta \mathbf{u} + \alpha \delta \mathbf{u} \cdot \mathbf{u}_a + \delta \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \delta \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} + \rho C_p \delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T T_a \Big] \\
&M^{(d_f)} \,\mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \Big\{ \tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta \mathbf{u})} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \\
&+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \Big[\rho \left(\delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta \mathbf{u} \right) + \nabla_\Gamma^{(d_f)} \delta p + \alpha \delta \mathbf{u} \Big] \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \\
&+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f;\delta \mathbf{u})} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \\
&\left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \delta \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) - \tau_{LST,\Gamma}^{(d_f;\delta \mathbf{u})} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \\
&\left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) - \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) \\
&- \tau_{LST,\Gamma}^{(d_f)} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\rho C_p \delta \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) \Big\} M^{(d_f)} \,\mathrm{d}\Sigma = 0,
\end{aligned} \tag{S-146}
$$

the first order variational of the augmented Lagrangian to γ_f can be set to be zero as

$$\begin{aligned}
&\int_{\Sigma_D} \bigg(\frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \mathbf{u}_a \delta\gamma_f + \frac{\partial k}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T \delta\gamma_f + \rho \frac{\partial C_p}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T T_a \delta\gamma_f \\
&+ \frac{\partial k}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \nabla_\Gamma^{(d_f)} T \cdot \nabla_\Gamma^{(d_f)} T_a \delta\gamma_f + r_f^2 \nabla_\Gamma^{(d_f)} \delta\gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \delta\gamma_f \gamma_{fa} \bigg) M^{(d_f)} \,\mathrm{d}\Sigma \\
&- \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma \cap \Sigma_D} \Bigg\{ \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) - \Bigg(\frac{\partial \tau_{LST,\Gamma}^{(d_f)}}{\partial C_p} \frac{\partial C_p}{\partial \gamma_p} \\
&+ \frac{\partial \tau_{LST,\Gamma}^{(d_f)}}{\partial k} \frac{\partial k}{\partial \gamma_p} \Bigg) \frac{\partial \gamma_p}{\partial \gamma_f} \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) - \tau_{LST,\Gamma}^{(d_f)} \rho \frac{\partial C_p}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \\
&\bigg[\left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T \right) \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) + \left(\rho C_p \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T - Q \right) \\
&\left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} T_a \right) \bigg] \Bigg\} \delta\gamma_f M^{(d_f)} \,\mathrm{d}\Sigma = 0,
\end{aligned} \tag{S-147}$$

and the first order variational of the augmented Lagrangian to d_f can be set to be zero as

$$
\begin{aligned}
&\int_\Sigma \left(2f_{id,\Gamma}k\nabla_\Gamma^{(d_f;\delta d_f)}T\cdot\nabla_\Gamma^{(d_f)}T\right)M^{(d_f)} + f_{id,\Gamma}k\nabla_\Gamma^{(d_f)}T\cdot\nabla_\Gamma^{(d_f)}TM^{(d_f;\delta d_f)} \\
&+\Big[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\delta d_f)}\right)\mathbf{u}\cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{(d_f;\delta d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f;\delta d_f)}\mathbf{u}^\mathrm{T}\right):\left(\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}\mathbf{u}_a^\mathrm{T}\right) \\
&+\frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right):\left(\nabla_\Gamma^{(d_f;\delta d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f;\delta d_f)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{(d_f;\delta d_f)}\mathbf{u}_a \\
&- p_a\mathrm{div}_\Gamma^{(d_f;\delta d_f)}\mathbf{u} + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{(d_f;\delta d_f)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{(d_f;\delta d_f)}\Big]M^{(d_f)} + \Big[\rho\left(\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\right)\mathbf{u} \\
&\cdot\mathbf{u}_a + \frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right):\left(\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a \\
&- p_a\,\mathrm{div}_\Gamma^{(d_f)}\mathbf{u} + \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{(d_f)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{(d_f)}\Big]M^{(d_f;\delta d_f)} \\
&+\Big[\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\delta d_f)}T\right)T_a + k\nabla_\Gamma^{(d_f;\delta d_f)}T\cdot\nabla_\Gamma^{(d_f)}T_a + k\nabla_\Gamma^{(d_f)}T\cdot\nabla_\Gamma^{(d_f;\delta d_f)}T_a\Big] \\
&M^{(d_f)} + \Big[\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T - Q\right)T_a + k\nabla_\Gamma^{(d_f)}T\cdot\nabla_\Gamma^{(d_f)}T_a\Big]M^{(d_f;\delta d_f)} \\
&+ f_{id,\Gamma}r_f^2\left(\nabla_\Gamma^{(d_f;\delta d_f)}\gamma_f\cdot\nabla_\Gamma^{(d_f)}\gamma_{fa} + \nabla_\Gamma^{(d_f)}\gamma_f\cdot\nabla_\Gamma^{(d_f;\delta d_f)}\gamma_{fa}\right)M^{(d_f)} \\
&+ f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{(d_f)}\gamma_f\cdot\nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right)M^{(d_f;\delta d_f)} \\
&+ r_m^2\nabla_\Sigma\delta d_f\cdot\nabla_\Sigma d_{fa} + \delta d_f d_{fa}\,\mathrm{d}\Sigma \\
&- \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}p_a\right) \\
&M^{(d_f)} + \tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\delta d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f;\delta d_f)}p\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}p_a\right)M^{(d_f)} \\
&+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\Big[\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\delta d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f;\delta d_f)}p_a\Big]M^{(d_f)} \\
&+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}p_a\right)M^{(d_f;\delta d_f)} \\
&+ \tau_{LSp,\Gamma}^{(d_f;\delta d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right)M^{(d_f)} + \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f;\delta d_f)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right) \\
&M^{(d_f)} + \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f;\delta d_f)}\mathbf{u}_a\right)M^{(d_f)} + \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right) \\
&\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right)M^{(d_f;\delta d_f)} - \tau_{LST,\Gamma}^{(d_f;\delta d_f)}\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T-Q\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T_a\right)M^{(d_f)} \\
&- \tau_{LST,\Gamma}^{(d_f)}\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\delta d_f)}T\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T_a\right)M^{(d_f)} \\
&- \tau_{LST,\Gamma}^{(d_f)}\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T-Q\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\delta d_f)}T_a\right)M^{(d_f)} \\
&- \tau_{LST,\Gamma}^{(d_f)}\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T-Q\right)\left(\rho C_p\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}T_a\right)M^{(d_f;\delta d_f)}\,\mathrm{d}\Sigma = 0.
\end{aligned}
\tag{S-148}
$$

The constraints in Eqs. S-142 and S-144 are imposed to Eqs. S-145, S-146, S-147 and S-148. Then, the adjoint sensitivity of J_T is derived as

$$\delta\hat{J}_T = -\int_{\Sigma_D}\gamma_{fa}\delta\gamma M^{(d_f)}\,\mathrm{d}\Sigma - \int_\Sigma A_d d_{fa}\delta d_m\,\mathrm{d}\Sigma. \tag{S-149}$$

Without losing the arbitrariness of $\delta \mathbf{u}$, δp, $\delta \lambda$, δT, $\delta \gamma_f$, δd_f, $\delta \gamma$ and δd_m, one can set

$$\left.\begin{array}{l} \tilde{\mathbf{u}}_a = \delta \mathbf{u} \\ \tilde{p}_a = \delta p \\ \tilde{\lambda}_a = \delta \lambda \\ \tilde{T}_a = \delta T \\ \tilde{\gamma}_{fa} = \delta \gamma_f \\ \tilde{d}_{fa} = \delta d_f \\ \tilde{\gamma} = \delta \gamma \\ \tilde{d}_m = \delta d_m \end{array}\right\} \text{ with } \left\{\begin{array}{l} \forall \tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\ \forall \tilde{p}_a \in \mathcal{H}\left(\Sigma\right) \\ \forall \tilde{\lambda}_a \in \mathcal{L}^2\left(\Sigma\right) \\ \forall \tilde{T}_a \in \mathcal{H}\left(\Sigma\right) \\ \forall \tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right) \\ \forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right) \\ \forall \tilde{\gamma} \in \mathcal{L}^2\left(\Sigma_D\right) \\ \forall \tilde{d}_m \in \mathcal{L}^2\left(\Sigma\right) \end{array}\right. \tag{S-150}$$

for Eqs. S-145, S-146, S-147 and S-148 to derive the adjoint system composed of Eqs. S-135, S-136, S-138 and S-139.

S-6.16 Variational formulations of adjoint equations for dissipation power in Eq. 32

In Eq. 38, the adjoint variables γ_{fa} and d_{fa} are derived by sequentially solving the variational formulation for the adjoint equations of the surface Navier-Stokes equations

$$\left\{\begin{array}{l}
\text{Find} \left\{\begin{array}{l} \mathbf{u}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \text{ with } \mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\ p_a \in \mathcal{H}\left(\Sigma\right) \\ \lambda_a \in \mathcal{L}^2\left(\Sigma\right) \text{ with } \lambda_a = 0 \text{ at } \forall \mathbf{x} \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \end{array}\right. \\
\text{for} \left\{\begin{array}{l} \forall \tilde{\mathbf{u}}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\ \forall \tilde{p}_a \in \mathcal{H}\left(\Sigma\right) \\ \tilde{\lambda}_a \in \mathcal{L}^2\left(\Sigma\right) \end{array}\right. \text{, such that} \\
\int_\Sigma \Big\{ \eta \left(\nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a + \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) + 2\alpha \mathbf{u} \cdot \tilde{\mathbf{u}}_a + \rho \Big[\left(\tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} \right) \mathbf{u} \\
+ \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \tilde{\mathbf{u}}_a \Big] \cdot \mathbf{u}_a + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a + \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) - \tilde{p}_a \\
\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a + \alpha \tilde{\mathbf{u}}_a \cdot \mathbf{u}_a + \tilde{\lambda}_a \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \tilde{\mathbf{u}}_a \cdot \mathbf{n}_\Gamma^{(d_f)} \Big\} M^{(d_f)} \,\mathrm{d}\Sigma \\
- \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \Big\{ \tau_{LS\mathbf{u},\Gamma}^{(d_f;\tilde{\mathbf{u}}_a)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \\
+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \Big[\rho \left(\tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a \right) + \nabla_\Gamma^{(d_f)} \tilde{p}_a + \alpha \tilde{\mathbf{u}}_a \Big] \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \\
+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha \mathbf{u} \right) \cdot \left(\rho \tilde{\mathbf{u}}_a \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f;\tilde{\mathbf{u}}_a)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \\
\left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \tilde{\mathbf{u}}_a \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) \Big\} M^{(d_f)} \,\mathrm{d}\Sigma = 0
\end{array}\right. \tag{S-151}$$

and the variational formulations for the adjoint equations of the surface-PDE filters

$$\left\{\begin{array}{l}
\text{Find } \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \text{ for } \forall \tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right), \text{ such that} \\
\int_{\Sigma_D} \left[\left(\frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u}^2 + \frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \mathbf{u}_a \right) \tilde{\gamma}_{fa} + r_f^2 \nabla_\Gamma^{(d_f)} \tilde{\gamma}_{fa} \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \tilde{\gamma}_{fa} \gamma_{fa} \right] M^{(d_f)} \,\mathrm{d}\Sigma \\
- \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma \cap \Sigma_D} \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \frac{\partial \alpha}{\partial \gamma_p} \frac{\partial \gamma_p}{\partial \gamma_f} \mathbf{u} \cdot \left(\rho \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \tilde{\gamma}_{fa} M^{(d_f)} \,\mathrm{d}\Sigma = 0
\end{array}\right. \tag{S-152}$$

and

$$
\begin{cases}
\text{Find } d_{fa} \in \mathcal{H}(\Sigma) \text{ for } \forall \tilde{d}_{fa} \in \mathcal{H}(\Sigma), \text{ such that} \\
\int_\Sigma \Big[\eta \left(\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u} + \nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) + \rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}\cdot\mathbf{u}_a \\
+ \frac{\eta}{2}\left(\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u} + \nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)}\mathbf{u}_a + \nabla_\Gamma^{(d_f)}\mathbf{u}_a^\mathrm{T}\right) + \frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) \\
: \left(\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}_a + \nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u} + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{(d_f;\tilde{d}_{fa})} \\
+ \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{(d_f;\tilde{d}_{fa})} + f_{id,\Gamma}r_f^2\left(\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\gamma_f\cdot\nabla_\Gamma^{(d_f)}\gamma_{fa} + \nabla_\Gamma^{(d_f)}\gamma_f\cdot\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\gamma_{fa}\right)\Big] M^{(d_f)} \\
+ \Big[\frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) + \alpha\mathbf{u}^2 + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\right)\mathbf{u}\cdot\mathbf{u}_a \\
+ \frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)}\mathbf{u}_a + \nabla_\Gamma^{(d_f)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{(d_f)}\mathbf{u} \\
+ \alpha\mathbf{u}\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{(d_f)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{(d_f)} + f_{id,\Gamma}\Big(r_f^2\nabla_\Gamma^{(d_f)}\gamma_f\cdot\nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} \\
- \gamma\gamma_{fa}\Big)\Big] M^{(d_f;\tilde{d}_{fa})} + r_m^2\nabla_\Sigma d_{fa}\cdot\nabla_\Sigma\tilde{d}_{fa} + d_{fa}\tilde{d}_{fa}\,\mathrm{d}\Sigma \\
- \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\Big[\tau_{LS\mathbf{u},\Gamma}^{(d_f;\tilde{d}_{fa})}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}p + \alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a + \nabla_\Gamma^{(d_f)}p_a\right) \\
+ \tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u} + \nabla_\Gamma^{(d_f;\tilde{d}_{fa})}p\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a + \nabla_\Gamma^{(d_f)}p_a\right) + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \\
\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}p + \alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}_a + \nabla_\Gamma^{(d_f;\tilde{d}_{fa})}p_a\right) + \tau_{LSp,\Gamma}^{(d_f;\tilde{d}_{fa})} \\
\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right) + \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right) + \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right) \\
\left(\mathrm{div}_\Gamma^{(d_f;\tilde{d}_{fa})}\mathbf{u}_a\right)\Big] M^{(d_f)} + \Big[\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}p + \alpha\mathbf{u}\right)\cdot\Big(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a \\
+ \nabla_\Gamma^{(d_f)}p_a\Big) + \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right)\Big] M^{(d_f;\tilde{d}_{fa})}\,\mathrm{d}\Sigma = 0.
\end{cases}
\tag{S-153}
$$

S-6.17 Adjoint analysis for constraint of dissipation power in Eq. 36

Based on the variational formulations of the surface Navier-Stokes equations in Eq. S-125 and the surface-PDE filters in Eqs. S-73 and S-74, the augmented Lagrangian of the dissipation power Φ in Eq. S-132 can be derived as

$$
\begin{split}
\hat{\Phi} = \int_\Sigma \Big[&\frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) + \alpha\mathbf{u}^2 + \rho\left(\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\right)\mathbf{u}\cdot\mathbf{u}_a \\
&+ \frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right) : \left(\nabla_\Gamma^{(d_f)}\mathbf{u}_a + \nabla_\Gamma^{(d_f)}\mathbf{u}_a^\mathrm{T}\right) - p\,\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a - p_a\mathrm{div}_\Gamma^{(d_f)}\mathbf{u} + \alpha\mathbf{u} \\
&\cdot\mathbf{u}_a + \lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{(d_f)} + \lambda_a\mathbf{u}\cdot\mathbf{n}_\Gamma^{(d_f)} + f_{id,\Gamma}\left(r_f^2\nabla_\Gamma^{(d_f)}\gamma_f\cdot\nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right)\Big] \\
&M^{(d_f)} + r_m^2\nabla_\Sigma d_f\cdot\nabla_\Sigma d_{fa} + d_f d_{fa} - A_d\left(d_m - \frac{1}{2}\right)d_{fa}\,\mathrm{d}\Sigma - \sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\tau_{LS\mathbf{u},\Gamma}^{(d_f)} \\
&\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u} + \nabla_\Gamma^{(d_f)}p + \alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a + \nabla_\Gamma^{(d_f)}p_a\right)M^{(d_f)} \\
&+ \tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right)M^{(d_f)}\,\mathrm{d}\Sigma,
\end{split}
\tag{S-154}
$$

where $\hat{\Phi}$ is the augmented lagrangian of Φ; and the adjoint variables satisfy

$$\left.\begin{array}{l}\mathbf{u}_a \in \left(\mathcal{H}\left(\Sigma\right)\right)^3 \\ p_a \in \mathcal{H}\left(\Sigma\right) \\ \lambda_a \in \mathcal{L}^2\left(\Sigma\right) \\ \gamma_{fa} \in \mathcal{H}\left(\Sigma_D\right) \\ d_{fa} \in \mathcal{H}\left(\Sigma\right)\end{array}\right\} \text{ with } \begin{cases}\mathbf{u}_a = \mathbf{0} \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma} \\ \lambda_a = 0 \text{ at } \forall \mathbf{x}_\Sigma \in l_{v,\Sigma} \cup l_{v_0,\Sigma}\end{cases}. \tag{S-155}$$

Based on the related results in Section 2, the first order variational of $\hat{\Phi}$ can be derived as

$$\begin{aligned}
\delta\hat{\Phi} = & \int_\Sigma \bigg\{ \eta \left(\nabla_\Gamma^{(d_f)} \delta\mathbf{u} + \nabla_\Gamma^{(d_f)} \delta\mathbf{u}^\mathrm{T} \right) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) + \eta \Big(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}^\mathrm{T} \Big) \\
& : \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) + 2\alpha \mathbf{u} \cdot \delta\mathbf{u} + \frac{\partial\alpha}{\partial\gamma_p} \frac{\partial\gamma_p}{\partial\gamma_f} \mathbf{u}^2 \delta\gamma_f + \rho \Big(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} \\
& + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta\mathbf{u} \Big) \cdot \mathbf{u}_a + \frac{\eta}{2} \Big(\nabla_\Gamma^{(d_f)} \delta\mathbf{u} + \nabla_\Gamma^{(d_f)} \delta\mathbf{u}^\mathrm{T} \Big) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) \\
& + \frac{\eta}{2} \Big(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}^\mathrm{T} \Big) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) + \frac{\eta}{2} \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) \\
& : \left(\nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a^\mathrm{T} \right) - \delta p \, \mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p \, \mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u} \\
& - p_a \mathrm{div}_\Gamma^{(d_f)} \delta\mathbf{u} + \frac{\partial\alpha}{\partial\gamma_p} \frac{\partial\gamma_p}{\partial\gamma_f} \mathbf{u} \cdot \mathbf{u}_a \delta\gamma_f + \alpha \delta\mathbf{u} \cdot \mathbf{u}_a + \delta\lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda \mathbf{u}_a \cdot \mathbf{n}_\Gamma^{(d_f;\delta d_f)} \\
& + \lambda_a \delta\mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f;\delta d_f)} + f_{id,\Gamma} \Big[r_f^2 \Big(\nabla_\Gamma^{(d_f)} \delta\gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \nabla_\Gamma^{(d_f;\delta d_f)} \gamma_f \\
& \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \gamma_{fa} \Big) + \delta\gamma_f \gamma_{fa} - \delta\gamma \gamma_{fa} \Big] \bigg\} M^{(d_f)} + \Big[\frac{\eta}{2} \Big(\nabla_\Gamma^{(d_f)} \mathbf{u} \\
& + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \Big) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \right) + \alpha \mathbf{u}^2 + \rho \left(\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \right) \mathbf{u} \cdot \mathbf{u}_a + \frac{\eta}{2} \Big(\nabla_\Gamma^{(d_f)} \mathbf{u} \\
& + \nabla_\Gamma^{(d_f)} \mathbf{u}^\mathrm{T} \Big) : \left(\nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} \mathbf{u}_a^\mathrm{T} \right) - p \, \mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a - p_a \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} + \alpha \mathbf{u} \cdot \mathbf{u}_a + \lambda \mathbf{u}_a \\
& \cdot \mathbf{n}_\Gamma^{(d_f)} + \lambda_a \mathbf{u} \cdot \mathbf{n}_\Gamma^{(d_f)} + f_{id,\Gamma} \cdot \left(r_f^2 \nabla_\Gamma^{(d_f)} \gamma_f \cdot \nabla_\Gamma^{(d_f)} \gamma_{fa} + \gamma_f \gamma_{fa} - \gamma \gamma_{fa} \right) \Big] M^{(d_f;\delta d_f)} \\
& + r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa} - A_d \delta d_m d_{fa} \, \mathrm{d}\Sigma - \sum_{E_\Sigma \in \mathcal{E}_\Sigma} \int_{E_\Sigma} \bigg\{ \left(\tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta d_f)} + \tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta\mathbf{u})} \right) \\
& \left(\rho\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha\mathbf{u} \right) \cdot \left(\rho\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \Big[\rho \Big(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} \\
& + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \delta\mathbf{u} \Big) + \nabla_\Gamma^{(d_f;\delta d_f)} p + \nabla_\Gamma^{(d_f)} \delta p + \frac{\partial\alpha}{\partial\gamma_p} \frac{\partial\gamma_p}{\partial\gamma_f} \mathbf{u} \delta\gamma_f + \alpha \delta\mathbf{u} \Big] \\
& \cdot \left(\rho\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) + \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \left(\rho\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha\mathbf{u} \right) \\
& \cdot \left[\rho \left(\delta\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \mathbf{u} \cdot \nabla_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a \right) + \nabla_\Gamma^{(d_f;\delta d_f)} p_a \right] + \left(\tau_{LSp,\Gamma}^{(d_f;\delta d_f)} + \tau_{LSp,\Gamma}^{(d_f;\delta\mathbf{u})} \right) \\
& \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f)} \rho \left(\mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u} + \mathrm{div}_\Gamma^{(d_f)} \delta\mathbf{u} \right) \\
& \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f;\delta d_f)} \mathbf{u}_a \right) \bigg\} M^{(d_f)} \\
& + \bigg\{ \tau_{LS\mathbf{u},\Gamma}^{(d_f)} \Big(\rho\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u} + \nabla_\Gamma^{(d_f)} p + \alpha\mathbf{u} \Big) \cdot \left(\rho\mathbf{u} \cdot \nabla_\Gamma^{(d_f)} \mathbf{u}_a + \nabla_\Gamma^{(d_f)} p_a \right) \\
& + \tau_{LSp,\Gamma}^{(d_f)} \left(\rho \mathrm{div}_\Gamma^{(d_f)} \mathbf{u} \right) \left(\mathrm{div}_\Gamma^{(d_f)} \mathbf{u}_a \right) \bigg\} M^{(d_f;\delta d_f)} \, \mathrm{d}\Sigma
\end{aligned} \tag{S-156}$$

with the satisfication of the constraints in Eq. S-155 and

$$\left.\begin{aligned}&\delta\mathbf{u}\in\left(\mathcal{H}\left(\Sigma\right)\right)^3\\&\delta p\in\mathcal{H}\left(\Sigma\right)\\&\delta\lambda\in\mathcal{L}^2\left(\Sigma\right)\\&\delta\gamma_f\in\mathcal{H}\left(\Sigma_D\right)\\&\delta\gamma\in\mathcal{L}^2\left(\Sigma_D\right)\\&\delta d_f\in\mathcal{H}\left(\Sigma\right)\\&\delta d_m\in\mathcal{L}^2\left(\Sigma\right)\end{aligned}\right\}\text{ with }\begin{cases}\delta\mathbf{u}=\mathbf{0}\text{ at }\forall\mathbf{x}\in l_{v,\Sigma}\cup l_{v_0,\Sigma}\\\delta\lambda=0\text{ at }\forall\mathbf{x}\in l_{v,\Sigma}\cup l_{v_0,\Sigma}\end{cases}. \tag{S-157}$$

According to the Karush-Kuhn-Tucker conditions of the PDE constrained optimization problem, the first order variational of the augmented Lagrangian to $\mathbf{u}$, p and λ can be set to be zero as

$$\begin{split}&\int_\Sigma\left\{\eta\left(\nabla_\Gamma^{(d_f)}\delta\mathbf{u}+\nabla_\Gamma^{(d_f)}\delta\mathbf{u}^\mathrm{T}\right):\left(\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}\mathbf{u}^\mathrm{T}\right)+2\alpha\mathbf{u}\cdot\delta\mathbf{u}+\rho\left[\left(\delta\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\right)\mathbf{u}\right.\right.\\&+\left.\left(\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\right)\delta\mathbf{u}\right]\cdot\mathbf{u}_a+\frac{\eta}{2}\left(\nabla_\Gamma^{(d_f)}\delta\mathbf{u}+\nabla_\Gamma^{(d_f)}\delta\mathbf{u}^\mathrm{T}\right):\left(\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}\mathbf{u}_a^\mathrm{T}\right)\\&\left.-\delta p\,\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a-p_a\mathrm{div}_\Gamma^{(d_f)}\delta\mathbf{u}+\alpha\delta\mathbf{u}\cdot\mathbf{u}_a+\delta\lambda\mathbf{u}_a\cdot\mathbf{n}_\Gamma^{(d_f)}+\lambda_a\delta\mathbf{u}\cdot\mathbf{n}_\Gamma^{(d_f)}\right\}M^{(d_f)}\,\mathrm{d}\Sigma\\&-\sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\left\{\tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta\mathbf{u})}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}p_a\right)\right.\\&+\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left[\rho\left(\delta\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}+\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\delta\mathbf{u}\right)+\nabla_\Gamma^{(d_f)}\delta p+\alpha\delta\mathbf{u}\right]\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}p_a\right)\\&+\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}+\nabla_\Gamma^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\left(\rho\delta\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a\right)+\tau_{LSp,\Gamma}^{(d_f;\delta\mathbf{u})}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}\right)\\&\left.\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right)+\tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_\Gamma^{(d_f)}\delta\mathbf{u}\right)\left(\mathrm{div}_\Gamma^{(d_f)}\mathbf{u}_a\right)\right\}M^{(d_f)}\,\mathrm{d}\Sigma=0,\end{split} \tag{S-158}$$

the first order variational of the augmented Lagrangian to the variable γ_f can be set to be zero as

$$\begin{split}&\int_{\Sigma_D}\left(\frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}^2\delta\gamma_f+\frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\mathbf{u}_a\delta\gamma_f+r_f^2\nabla_\Gamma^{(d_f)}\delta\gamma_f\cdot\nabla_\Gamma^{(d_f)}\gamma_{fa}+\delta\gamma_f\gamma_{fa}\right)M^{(d_f)}\,\mathrm{d}\Sigma\\&-\sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma\cap\Sigma_D}\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\frac{\partial\alpha}{\partial\gamma_p}\frac{\partial\gamma_p}{\partial\gamma_f}\mathbf{u}\cdot\left(\rho\mathbf{u}\cdot\nabla_\Gamma^{(d_f)}\mathbf{u}_a+\nabla_\Gamma^{(d_f)}p_a\right)\delta\gamma_fM^{(d_f)}\,\mathrm{d}\Sigma=0,\end{split} \tag{S-159}$$

and the first order variational of the augmented Lagrangian to the variable d_f can be set to be zero as

$$\int_{\Sigma}\left[\eta\left(\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}^{\mathrm{T}}\right):\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}\mathbf{u}^{\mathrm{T}}\right)+\rho\left(\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f;\delta d_f)}\right)\mathbf{u}\cdot\mathbf{u}_a\right.$$
$$+\frac{\eta}{2}\left(\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}^{\mathrm{T}}\right):\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a^{\mathrm{T}}\right)+\frac{\eta}{2}\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}\mathbf{u}^{\mathrm{T}}\right)$$
$$:\left(\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}_a^{\mathrm{T}}\right)-p\,\mathrm{div}_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}_a-p_a\mathrm{div}_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}+\lambda\mathbf{u}_a\cdot\mathbf{n}_{\Gamma}^{(d_f;\delta d_f)}$$
$$\left.+\lambda_a\mathbf{u}\cdot\mathbf{n}_{\Gamma}^{(d_f;\delta d_f)}+f_{id,\Gamma}r_f^2\left(\nabla_{\Gamma}^{(d_f;\delta d_f)}\gamma_f\cdot\nabla_{\Gamma}^{(d_f)}\gamma_{fa}+\nabla_{\Gamma}^{(d_f)}\gamma_f\cdot\nabla_{\Gamma}^{(d_f;\delta d_f)}\gamma_{fa}\right)\right]M^{(d_f)}$$
$$+\left[\frac{\eta}{2}\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}\mathbf{u}^{\mathrm{T}}\right):\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}\mathbf{u}^{\mathrm{T}}\right)+\alpha\mathbf{u}^2+\rho\left(\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\right)\mathbf{u}\cdot\mathbf{u}_a\right.$$
$$+\frac{\eta}{2}\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}\mathbf{u}^{\mathrm{T}}\right):\left(\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a^{\mathrm{T}}\right)-p\,\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}_a-p_a\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}$$
$$+\alpha\mathbf{u}\cdot\mathbf{u}_a+\lambda\mathbf{u}_a\cdot\mathbf{n}_{\Gamma}^{(d_f)}+\lambda_a\mathbf{u}\cdot\mathbf{n}_{\Gamma}^{(d_f)}+f_{id,\Gamma}\left(r_f^2\nabla_{\Gamma}^{(d_f)}\gamma_f\cdot\nabla_{\Gamma}^{(d_f)}\gamma_{fa}+\gamma_f\gamma_{fa}\right.$$
$$\left.\left.-\gamma\gamma_{fa}\right)\right]M^{(d_f;\delta d_f)}+r_m^2\nabla_{\Sigma}\delta d_f\cdot\nabla_{\Sigma}d_{fa}+\delta d_f d_{fa}\,\mathrm{d}\Sigma$$
$$-\sum_{E_\Sigma\in\mathcal{E}_\Sigma}\int_{E_\Sigma}\left[\tau_{LS\mathbf{u},\Gamma}^{(d_f;\delta d_f)}\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f)}p_a\right)\right.$$
$$+\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f;\delta d_f)}p\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f)}p_a\right)$$
$$+\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}p+\alpha\mathbf{u}\right)\cdot\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f;\delta d_f)}p_a\right)$$
$$+\tau_{LSp,\Gamma}^{(d_f;\delta d_f)}\left(\rho\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}_a\right)+\tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}\right)\left(\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}_a\right)$$
$$\left.+\tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_{\Gamma}^{(d_f;\delta d_f)}\mathbf{u}_a\right)\right]M^{(d_f)}+\left[\tau_{LS\mathbf{u},\Gamma}^{(d_f)}\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\mathbf{u}+\nabla_{\Gamma}^{(d_f)}p+\alpha\mathbf{u}\right)\right.$$
$$\left.\cdot\left(\rho\mathbf{u}\cdot\nabla_{\Gamma}^{(d_f)}\mathbf{u}_a+\nabla_{\Gamma}^{(d_f)}p_a\right)+\tau_{LSp,\Gamma}^{(d_f)}\left(\rho\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}\right)\left(\mathrm{div}_{\Gamma}^{(d_f)}\mathbf{u}_a\right)\right]M^{(d_f;\delta d_f)}\,\mathrm{d}\Sigma=0. \tag{S-160}$$

The constraints in Eqs. S-155 and S-157 are imposed to Eqs. S-158, S-159 and S-160. Then, the adjoint sensitivity of Φ is derived as

$$\delta\hat{\Phi}=-\int_{\Sigma_D}\delta\gamma\gamma_{fa}M^{(d_f)}\,\mathrm{d}\Sigma-\int_{\Sigma}A_d\delta d_m d_{fa}\,\mathrm{d}\Sigma. \tag{S-161}$$

Without losing the arbitrariness of $\delta\mathbf{u}$, δp, $\delta\lambda$, $\delta\gamma_f$, δd_f, $\delta\gamma$ and δd_m, one can set

$$\left.\begin{aligned}\tilde{\mathbf{u}}_a&=\delta\mathbf{u}\\ \tilde{p}_a&=\delta p\\ \tilde{\lambda}_a&=\delta\lambda\\ \tilde{\gamma}_{fa}&=\delta\gamma_f\\ \tilde{d}_{fa}&=\delta d_f\\ \tilde{\gamma}&=\delta\gamma\\ \tilde{d}_m&=\delta d_m\end{aligned}\right\}\text{ with }\left\{\begin{aligned}&\forall\tilde{\mathbf{u}}_a\in\left(\mathcal{H}\left(\Sigma\right)\right)^3\\ &\forall\tilde{p}_a\in\mathcal{H}\left(\Sigma\right)\\ &\forall\tilde{\lambda}_a\in\mathcal{L}^2\left(\Sigma\right)\\ &\forall\tilde{\gamma}_{fa}\in\mathcal{H}\left(\Sigma_D\right)\\ &\forall\tilde{d}_{fa}\in\mathcal{H}\left(\Sigma\right)\\ &\forall\tilde{\gamma}\in\mathcal{L}^2\left(\Sigma_D\right)\\ &\forall\tilde{d}_m\in\mathcal{L}^2\left(\Sigma\right)\end{aligned}\right. \tag{S-162}$$

for Eqs. S-158, S-159 and S-160 to derive the adjoint system composed of Eqs. S-151, S-152 and S-153.

S-6.18 Variational formulations of adjoint equations for area fraction in Eq. 34

In Eq. 40, the adjoint variables γ_{fa} and d_{fa} are derived by sequentially solving the variational formulations for the adjoint equations of the surface-PDE filters:

$$\left\{\begin{aligned}&\text{Find }\gamma_{fa}\mathcal{H}\left(\Sigma_D\right)\ \text{ for }\forall\tilde{\gamma}_{fa}\mathcal{H}\left(\Sigma_D\right),\ \text{ such that}\\ &\int_{\Sigma_D}\left(\frac{\partial\gamma_p}{\partial\gamma_f}\tilde{\gamma}_{fa}+r_f^2\nabla_{\Gamma}^{(d_f)}\gamma_{fa}\cdot\nabla_{\Gamma}^{(d_f)}\tilde{\gamma}_{fa}+\gamma_{fa}\tilde{\gamma}_{fa}\right)M^{(d_f)}\,\mathrm{d}\Sigma=0\end{aligned}\right. \tag{S-163}$$

and

$$\begin{cases}\text{Find } d_{fa}\mathcal{H}(\Sigma) \text{ for } \forall\tilde{d}_{fa}\mathcal{H}(\Sigma)\text{, such that}\\ \displaystyle\int_\Sigma f_{id,\Gamma} r_f^2 \left(\nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f;\tilde{d}_{fa})}\gamma_{fa}\right) M^{(d_f)}\\ + f_{id,\Gamma}\left(\gamma_p + r_f^2\nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right) M^{(d_f;\tilde{d}_{fa})}\\ + r_m^2 \nabla_\Sigma d_{fa} \cdot \nabla_\Sigma \tilde{d}_{fa} + d_{fa}\tilde{d}_{fa}\,\mathrm{d}\Sigma = 0.\end{cases} \tag{S-164}$$

In Eq. 41, the adjoint variable d_{fa} is derived by solving the variational formulation for the adjoint equation of the surface-PDE filter for the implicit 2-manifold:

$$\begin{cases}\text{Find } d_{fa}\mathcal{H}(\Sigma) \text{ for } \forall\tilde{d}_{fa}\mathcal{H}(\Sigma)\text{, such that}\\ \displaystyle\int_\Sigma f_{id,\Gamma} M^{(d_f;\tilde{d}_{fa})} + r_m^2 \nabla_\Sigma d_{fa} \cdot \nabla_\Sigma \tilde{d}_{fa} + d_{fa}\tilde{d}_{fa}\,\mathrm{d}\Sigma = 0.\end{cases} \tag{S-165}$$

S-6.19 Adjoint analysis for area constraint in Eq. 36

The adjoint sensitivity of the area fraction of the surface structure can be derived from that of the area of the surface structure and the area of the implicit 2-manifold. The adjoint analysis in this section is implemented for those two areas.

S-6.19.1 Adjoint analysis for area of surface structure

Based on the variational formulations of the surface-PDE filters in Eqs. S-73 and S-74, the augmented Lagrangian of the area of the surface structure can be derived as

$$\begin{split}\widehat{s\,|\Gamma_D|} = &\int_\Sigma f_{id,\Gamma}\left(\gamma_p + r_f^2\nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right) M^{(d_f)}\\ &+ r_m^2 \nabla_\Sigma d_f \cdot \nabla_\Sigma d_{fa} + d_f d_{fa} - A_d\left(d_m - \frac{1}{2}\right) d_{fa}\,\mathrm{d}\Sigma,\end{split} \tag{S-166}$$

where $\widehat{s\,|\Gamma_D|}$ is the augmented lagrangian of $s\,|\Gamma_D|$; and the adjoint variables satisfy

$$\begin{cases}\gamma_{fa} \in \mathcal{H}(\Sigma_D)\\ d_{fa} \in \mathcal{H}(\Sigma)\end{cases}. \tag{S-167}$$

Based on the related results in Section 2, the first order variational of $\widehat{s\,|\Gamma_D|}$ can be derived as

$$\begin{split}\delta\widehat{s\,|\Gamma_D|} = &\int_\Sigma f_{id,\Gamma}\Big[\frac{\partial\gamma_p}{\partial\gamma_f}\delta\gamma_f + r_f^2\Big(\nabla_\Gamma^{(d_f)}\delta\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \nabla_\Gamma^{(d_f;\delta d_f)}\gamma_f\\ &\cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f;\delta d_f)}\gamma_{fa}\Big) + \delta\gamma_f\gamma_{fa} - \delta\gamma\gamma_{fa}\Big] M^{(d_f)}\\ &+ f_{id,\Gamma}\Big(\gamma_p + r_f^2\nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\Big) M^{(d_f;\delta d_f)}\\ &+ r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa} - A_d \delta d_m d_{fa}\,\mathrm{d}\Sigma\end{split} \tag{S-168}$$

with the satisfication of Eq. S-167 and

$$\begin{cases}\delta\gamma_f \in \mathcal{H}(\Sigma_D)\\ \delta\gamma \in \mathcal{L}^2(\Sigma_D)\\ \delta d_f \in \mathcal{H}(\Sigma)\\ \delta d_m \in \mathcal{L}^2(\Sigma)\end{cases}. \tag{S-169}$$

According to the Karush-Kuhn-Tucker conditions of the PDE constrained optimization problem, the first order variational of the augmented Lagrangian to γ_f can be set to be zero as

$$\int_{\Sigma_D}\left(\frac{\partial\gamma_p}{\partial\gamma_f}\delta\gamma_f + r_f^2\nabla_\Gamma^{(d_f)}\delta\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \delta\gamma_f\gamma_{fa}\right) M^{(d_f)}\,\mathrm{d}\Sigma = 0, \tag{S-170}$$

and the first order variational of the augmented Lagrangian to the variable d_f can be set to be zero as

$$\begin{split}&\int_\Sigma f_{id,\Gamma} r_f^2 \left(\nabla_\Gamma^{(d_f;\delta d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f;\delta d_f)}\gamma_{fa}\right) M^{(d_f)}\\ &+ f_{id,\Gamma}\left(\gamma_p + r_f^2\nabla_\Gamma^{(d_f)}\gamma_f \cdot \nabla_\Gamma^{(d_f)}\gamma_{fa} + \gamma_f\gamma_{fa} - \gamma\gamma_{fa}\right) M^{(d_f;\delta d_f)}\\ &+ r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa}\,\mathrm{d}\Sigma = 0.\end{split} \tag{S-171}$$

The constraints in Eqs. S-167 and S-169 are imposed to Eqs. S-170 and S-171. Then, the adjoint sensitivity of $s\left|\Gamma_D\right|$ is derived as

$$\delta \widehat{s\left|\Gamma_D\right|} = -\int_{\Sigma_D} \delta\gamma \gamma_{fa} M^{\left(d_f\right)} \,\mathrm{d}\Sigma - \int_{\Sigma} A_d \delta d_m d_{fa} \,\mathrm{d}\Sigma. \tag{S-172}$$

Without losing the arbitrariness of $\delta\gamma_f$, δd_f, $\delta\gamma$ and δd_m, one can set

$$\left.\begin{aligned} \tilde{\gamma}_{fa} &= \delta\gamma_f \\ \tilde{d}_{fa} &= \delta d_f \\ \tilde{\gamma} &= \delta\gamma \\ \tilde{d}_m &= \delta d_m \end{aligned}\right\} \text{ with } \begin{cases} \forall \tilde{\gamma}_{fa} \in \mathcal{H}\left(\Sigma_D\right) \\ \forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right) \\ \forall \tilde{\gamma} \in \mathcal{L}^2\left(\Sigma_D\right) \\ \forall \tilde{d}_m \in \mathcal{L}^2\left(\Sigma\right) \end{cases} \tag{S-173}$$

for Eqs. S-170 and S-171 to derive the adjoint system composed of Eqs. 40, S-163 and S-164.

S-6.19.2 Adjoint analysis for area of implicit 2-manifold

Based on the variational formulation of the surface-PDE filter in Eq. S-73, the augmented Lagrangian of the area of the implicit 2-manifold can be derived as

$$\widehat{\left|\Gamma_D\right|} = \int_{\Sigma} f_{id,\Gamma} M^{\left(d_f\right)} + r_m^2 \nabla_\Sigma d_f \cdot \nabla_\Sigma d_{fa} + d_f d_{fa} - A_d \left(d_m - \frac{1}{2}\right) d_{fa} \,\mathrm{d}\Sigma, \tag{S-174}$$

where $\widehat{\left|\Gamma_D\right|}$ is the augmented lagrangian of $\left|\Gamma_D\right|$; and the adjoint variables satisfy

$$d_{fa} \in \mathcal{H}\left(\Sigma\right). \tag{S-175}$$

Based on the related results in Section 2, the first order variational of $\widehat{\left|\Gamma_D\right|}$ can be derived as

$$\delta\widehat{\left|\Gamma_D\right|} = \int_{\Sigma} f_{id,\Gamma} M^{\left(d_f;\delta d_f\right)} + r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa} - A_d \delta d_m d_{fa} \,\mathrm{d}\Sigma \tag{S-176}$$

with the satisfication of Eq. S-175 and

$$\begin{cases} \delta d_f \in \mathcal{H}\left(\Sigma\right) \\ \delta d_m \in \mathcal{L}^2\left(\Sigma\right) \end{cases}. \tag{S-177}$$

According to the Karush-Kuhn-Tucker conditions of the PDE constrained optimization problem, the first order variational of the augmented Lagrangian to d_f can be set to be zero as

$$\int_{\Sigma} f_{id,\Gamma} M^{\left(d_f;\delta d_f\right)} + r_m^2 \nabla_\Sigma \delta d_f \cdot \nabla_\Sigma d_{fa} + \delta d_f d_{fa} \,\mathrm{d}\Sigma = 0. \tag{S-178}$$

The constraints in Eqs. S-175 and S-177 are imposed to Eq. S-178. Then, the adjoint sensitivity of $\left|\Gamma_D\right|$ is derived as

$$\delta\widehat{\left|\Gamma_D\right|} = \int_{\Sigma} -A_d \delta d_m d_{fa} \,\mathrm{d}\Sigma. \tag{S-179}$$

Without losing the arbitrariness of δd_f and δd_m, one can set

$$\left.\begin{aligned} \tilde{d}_{fa} &= \delta d_f \\ \tilde{d}_m &= \delta d_m \end{aligned}\right\} \text{ with } \begin{cases} \forall \tilde{d}_{fa} \in \mathcal{H}\left(\Sigma\right) \\ \forall \tilde{d}_m \in \mathcal{L}^2\left(\Sigma\right) \end{cases} \tag{S-180}$$

for Eqs. S-178 and S-179 to derive the adjoint system composed of Eqs. 41 and S-165.

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