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A Strongly-coupled Non-parametric Integral Boundary Layer Method for Aerodynamic Analysis with Free Transition

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The integral boundary layer (IBL) method with viscous-inviscid coupling is an effective tool for rapid aerodynamic design and analysis. However, existing IBL methods remain to be extended to general three-dimensional (3D) configurations. To this end, previous work proposed an IBL formulation using the discontinuous Galerkin (DG) finite element method (FEM) with strong viscous-inviscid coupling, which is non-parametric in the sense that the aerodynamic shape does not have to be explicitly parametrized by curvilinear coordinates. The current work builds on that strongly-coupled non-parametric IBL formulation, and further develops numerical discretization methods to enable flow transition modeling. Both a cut-cell-based fitted transition approach and a simple captured transition approach are presented and compared. In solving the nonlinear system of equations arising from free-transition problems, a strongly-coupled global Newton solver is adopted and augmented for solution robustness. Numerical results demonstrate favorable accuracy and robustness of the cut-cell fitted transition method compared to the captured transition methods. On the other hand, the captured transition approach allows for a more straightforward numerical implementation, but requires further improvement to achieve comparable reliability for aerodynamic analysis with free transition.

Nomenclature

$\mathbf{r}$	position vector	$\delta, \mathcal{A}, \mathcal{G}$	IBL primary unknowns
$\mathbf{q}$	velocity vector	x, y	global Cartesian coordinates
q	speed (= $ \mathbf{q} $)	ξ	local surface coordinate
ρ	density	$\hat{\mathbf{e}}$	local Cartesian basis vector
$\boldsymbol{\tau}$	shear stress vector	$s, \hat{\mathbf{s}}_1$	streamwise coordinate, basis vector
$\mathcal{D}$	dissipation integral	$\hat{\mathbf{t}}$	outward unit normal vector
$C_{\mathcal{D}}$	dissipation coefficient	$\hat{\mathbf{n}}$	unit surface normal vector
C_{f1}	skin-friction coefficient	$\tilde{\nabla}$	$\partial(\cdot)/\partial\xi \hat{\mathbf{e}}$
c_{τ}	shear stress coefficient	$(\cdot)_i$	inviscid quantity
δ_1^*	mass defect thickness	$(\cdot)_e$	viscous layer edge quantity
θ_{11}	momentum defect thickness	$(\cdot)_w$	wall quantity
θ_1^*	kinetic defect thickness	$(\cdot)_{\infty}$	freestream quantity
H	shape parameter $H = \delta_1^*/\theta_{11}$	$\hat{(\cdot)}$	unit vector
H^*	kinetic energy shape parameter $H^* = \theta_1^*/\theta_{11}$	$\overline{\overline{(\cdot)}}$	tensor

Scalars are in normal font, vectors are boldface, and tensors are boldface with double overbars. Other notations follow the nomenclature used in Ref. [1] or will be defined later where they first appear.

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I. Introduction

Computational fluid dynamics (CFD) has become a powerful and indispensable tool for aerodynamic design and analysis. Among various existing CFD methods, the integral boundary layer (IBL) method coupled with an inviscid solver, utilizing viscous-inviscid interaction (VII), boasts its rapid computational speed, convenient formulation, and multi-disciplinary compatibility.

The advantageous computational efficiency of the coupled IBL method is conducive to numerous design and optimization iterations that are impractically expensive when higher-fidelity methods are employed, such as Reynolds-averaged Navier-Stokes (RANS) solvers. Besides, the coupled IBL method can potentially help bootstrap its higher-fidelity counterparts by providing a lower-cost yet plausible initial solution. Also, flow transition problems have traditionally been better served by boundary layer methods [2, 3] owing to the convenient incorporation of established flow transition models, e.g. the linear flow instability theory, which are less amenable to the RANS formulation [4, 5]. Moreover, in fluid-structure interaction (FSI) problems, the aerostructural coupling using the IBL formulation via a displacement body model [6] is much simpler than RANS which typically requires re-meshing [7]. These benefits render the coupled IBL method a desirable tool for rapid medium-fidelity aerodynamic and aeroelastic analysis.

Well-established two-dimensional (2D) examples of the IBL method include MSES [2] and XFOIL [3]. However, such capability and reliability for three-dimensional (3D) applications is not yet available. The quasi-2D method, such as Boeing’s TRANAIR code [8, 9], stands as a viable intermediate approach, but falls short in fully 3D cases. As for traditional 3D boundary layer solvers, the dependence on curvilinear coordinates limits their applicability to complex geometries. This issue was later sidestepped by non-parametric IBL formulations [1, 10–14]. For example, continuing from Drela’s 3D IBL formulation [12], Zhang et al. [1, 14] proposed a discontinuous Galerkin (DG) finite element method (FEM) for discretizing the IBL equations. The non-parametric feature specifically refers to the independence of any explicit geometry parametrization using curvilinear coordinates. In addition, Ref. [1] presents a strong viscous-inviscid coupling scheme for solution robustness, flexible choice in the inviscid solver, and potential aerostructural extension.

The current work extends that of Ref. [1], and focuses on enabling flow transition modeling in the non-parametric DG IBL method. The understanding and management of flow transition bears significant importance in aerodynamic analysis and design [6, 15]. Among existing physical models for transition prediction, the e^N envelope method is a popular choice for its effectiveness and efficiency, and thus is adopted in the current work. The key challenge falls upon the numerical discretization to handle the solution-dependent interface identified by the free transition front in an accurate and robust manner. In tackling such a challenge, we develop and compare both “fitted” and “captured” transition formulations in the DG-FEM setting. While the captured approach conveniently lends itself to a plain DG FEM, the fitted transition is realized using a cut-cell DG method. Suitable and robust nonlinear solution techniques are also pursued in this work for solving the free-interface problem that arises from modeling flow transition. A strongly-coupled global Newton solver is adopted, with extensions including a line-search algorithm and under-relaxation. In addition, the turbulence closure model of Ref. [1] is augmented to account for the lag effect in the turbulent shear stress transport.

This paper concentrates on the capability of the current IBL formulation for aerodynamic analysis with free transition. It mainly deals with the challenges on the numerical methods, while the improvement of existing physical models (such as closure relations and profile families) will be considered separately. Also, as an example, we focus on 2D steady-state incompressible flows, and use a panel method as the inviscid solver. The current formulation is intended to be generalized for three-dimensional (3D) time-dependent applications, and coupling with other inviscid flow (e.g. potential flow and Euler solvers [16, 17]) and structural formulations (e.g. a hybrid shell model [18]) in future work.

In the following discussion, Section II first describes the viscous-inviscid coupling formulation, with a focus on the IBL formulation updates compared to Ref. [1]. Then, Section III and IV present the numerical discretization of the IBL problem with flow transition using a DG FEM, and the strongly-coupled solution procedure, respectively. The proposed methods are demonstrated on numerical test cases in Section V.

II. Viscous-Inviscid Formulation

This section briefly summarizes the key components of the viscous-inviscid formulation that Ref. [1] discusses in greater detail, and elaborates on the updates such as the turbulent closure and transition formulation.

A. Inviscid Formulation

The viscous-inviscid interaction scheme of this paper is intended to be flexible with various inviscid formulations, such as potential flow and Euler equations. As an example, we currently examine steady-state incompressible flows, for

which the inviscid flow field is governed by the following equation and boundary condition,

$$\nabla^2 \Phi = 0 \quad \text{subject to} \quad (\rho_i \mathbf{q}_i)_w \cdot \hat{\mathbf{n}}_w = \Lambda \quad (1)$$

Here, the unknown variable Φ is the velocity potential, and the flow velocity is $\mathbf{q}_i = \nabla \Phi$. The source term Λ models the displacement effect potentially originating from viscous-inviscid interaction, geometry changes (e.g. in FSI problems), and wall transpiration.

B. Integral Boundary Layer Formulation

The viscous flow field is governed by the IBL equations, derived in Ref. [1] and given as follows,

$$\frac{\partial \mathbf{p}}{\partial t} + m \frac{\partial \mathbf{q}_e}{\partial t} + \tilde{\nabla} \cdot \bar{\mathbf{P}} + (\tilde{\nabla} \mathbf{q}_e) \cdot \mathbf{M} - \tau_w = \mathbf{0} \quad (\text{momentum}) \quad (2)$$

$$\frac{\partial k}{\partial t} + m \frac{\partial (q_e^2)}{\partial t} + \tilde{\nabla} \cdot \mathbf{K} + \mathbf{D} \cdot \tilde{\nabla} (q_e^2) - 2 \mathcal{D} = 0 \quad (\text{kinetic energy}) \quad (3)$$

The edge velocity $\mathbf{q}_e$ (with magnitude q_e) is determined from the viscous-inviscid interaction. Integral defect quantities (including $\mathbf{p}, m, \bar{\mathbf{P}}, \mathbf{M}, k, \mathbf{K}, \mathbf{D}$), the wall shear stress vector τ_w , and the dissipation integral $\mathcal{D}$ are defined in Ref. [1]. They are parametrized by two primary variables $\{\delta, \mathcal{A}\}$ (i.e. the viscous layer thickness and the profile shape parameter, respectively) using closure models including velocity profiles and dissipation relations.

The IBL equations (2) and (3) apply to both laminar and turbulent flows, albeit using different closure models. The laminar closure follows Ref. [1]. Only changes regarding the turbulent and transition closures are described in the following discussion.

1. Turbulent Closure

The turbulent velocity profile from Ref. [1] is reused in the current formulation. As for the turbulent dissipation closure, while Ref. [1] assumes an equilibrium flow, the current formulation incorporates a non-equilibrium model to account for the lag effect in the turbulent shear stress transport.

The viscous dissipation depends on the shear stress τ , and is measured in terms of the dissipation integral $\mathcal{D}$, or the non-dimensional dissipation coefficient C_D . The turbulent shear stress profile is assumed to consist of an inner wall layer and an outer wake layer. Hence, the dissipation coefficient C_D comprises contributions from the inner and the outer parts as follows,

$$C_D = \underbrace{(C_{f1}/2) U_s}_{\text{inner}} + \underbrace{c_\tau (1 - U_s)}_{\text{outer}} \quad (4)$$

This expression was derived by Drela [19] using a slip velocity profile model with a normalized wall slip velocity U_s given below in (10). While the inner part responds almost instantaneously to local changes of flow properties (e.g. the wall shear stress τ_w), the evolution of the outer wake layer is modeled using a transport equation [19]. As a result, the outer-layer shear stress can “lag” behind the local velocity profile in both magnitude and direction (i.e. the in-plane flow angle) in a general 3D case. It suffices to consider only the magnitude lag for the current discussion of 2D flows.

The Reynolds shear stress predominates the dissipation effect in the outer layer, and is quantified using the shear stress coefficient defined as,

$$c_\tau \equiv \frac{\|\tau\|}{\rho_e q_e^2} = \frac{\left\| \rho \overline{\mathbf{q}' \mathbf{q}'^T} \cdot \hat{\mathbf{n}} \right\|}{\rho_e q_e^2} \approx \frac{q'^2}{q_e^2}, \quad q' \equiv \left\| \overline{\mathbf{q}' \cdot \mathbf{q}'} \right\|^{1/2} \quad (5)$$

under some suitable norm $\|\cdot\|$ (e.g. the L^∞ -norm across the shear layer thickness as employed by Green et al. [20]). The Reynolds-averaged quantities are denoted with an overline as $\overline{(\cdot)}$, and the velocity fluctuation is $\mathbf{q}'$. We note that c_τ constitutes a measure in a mean-flow sense, similar to other IBL integral defect quantities.

Based on the turbulent shear stress transport equations of Bradshaw et al. [21], Green et al. [20] derived the following steady-state lag equation for 2D flows,

$$\frac{\tilde{\delta}}{c_\tau} \frac{dc_\tau}{ds_1} = 5.6 \left((c_\tau)_{\text{eq}}^{1/2} - c_\tau^{1/2} \right) + 2 \left(\frac{\tilde{\delta}}{q_e} \frac{dq_e}{ds_1} \right)_{\text{eq}} - \frac{2\tilde{\delta}}{q_e} \frac{dq_e}{ds_1} \quad (6)$$

where $\tilde{\delta}$ denotes the conventional boundary layer thickness defined based on 99.5% of the edge speed, the subscript “eq” corresponds to equilibrium flows, and s_1 refers to the streamwise coordinate. Using the equilibrium pressure gradient parameter given in Ref. [1],

$$\left(\frac{\theta_{11}}{q_e} \frac{dq_e}{ds_1} \right)_{\text{eq}} = \left(\frac{C_{f1}}{2} - G_A^2 \right) \frac{1}{B_{\text{eq}} H} \quad (7)$$

and the following practical approximations in XFOIL [22],

$$\tilde{\delta} = \theta_{11} \min \left\{ 12, \left(3.15 + \frac{1.72}{H-1} \right) + \frac{\delta^*}{\theta_{11}} \right\}, \quad K_{\text{dl}} = \begin{cases} 1.0, & \text{boundary layer} \\ 0.9, & \text{wake} \end{cases} \quad (8)$$

a lag equation on c_τ is derived and written as follows,

$$\frac{\partial c_\tau}{\partial t} + \mathbf{q}_e \cdot \tilde{\nabla} c_\tau - \frac{q_e c_\tau}{\tilde{\delta}} \left[5.6 \left((c_\tau)_{\text{eq}}^{1/2} - c_\tau^{1/2} \right) \right] - \frac{2 q_e c_\tau}{B_{\text{eq}} \delta_1^*} \left[\frac{C_{f1}}{2} - \left(\frac{H-1}{A_{\text{eq}} K_{\text{dl}} H} \right)^2 \right] + 2 c_\tau \tilde{\nabla} \cdot \mathbf{q}_e = 0 \quad (9)$$

The equilibrium shear stress coefficient $(c_\tau)_{\text{eq}}$, and the normalized wall slip velocity U_s are defined as follows,

$$(c_\tau)_{\text{eq}} = \frac{H^*}{2} \frac{1}{1 - U_s} G_A^2 G_B, \quad U_s = \frac{H^*}{2} \left(1 - \frac{H-1}{H B_{\text{eq}}} \right), \quad G_A \equiv \frac{H-1}{A_{\text{eq}} H}, \quad G_B \equiv \frac{H-1}{B_{\text{eq}} H} \quad (10)$$

where A_{eq} and B_{eq} are the two parameters of the G - β locus of equilibrium boundary layers [1],

$$G = A_{\text{eq}} \sqrt{1 + B_{\text{eq}} \beta}, \quad G \approx \frac{1}{\sqrt{C_{f1}/2}} \frac{H-1}{H}, \quad \beta \approx -\frac{2}{C_{f1}} \frac{H \theta_{11}}{\mathbf{q}_e \cdot \hat{\mathbf{s}}_1} \frac{d(\mathbf{q}_e \cdot \hat{\mathbf{s}}_1)}{ds_1} \quad (G - \beta \text{ locus}) \quad (11)$$

The expressions of $(c_\tau)_{\text{eq}}$ and U_s are derived by matching the inner and outer terms of the expression (4) with those of the following dissipation coefficient for equilibrium boundary layers [1],

$$(C_D)_{\text{eq}} = \frac{H^*}{2} \left[\frac{C_{f1}}{2} (1 - G_B) + G_B G_A^2 \right] \quad (12)$$

The turbulent dissipation closure applies to not only wall boundary layers but also free wakes for which the skin friction coefficient C_{f1} is set to zero. Also, the expression (4) corresponds to a half of the whole viscous layer in the wake, and is doubled to give the actual dissipation coefficient C_D .

Moreover, for convenience, we define an alternative variable $\mathcal{G}$ as

$$\mathcal{G} \equiv \ln \frac{q'}{q_e} = \ln \left(c_\tau^{1/2} \right) \quad (13)$$

and transform the lag equation (9) into the following equivalent form,

$$\frac{\partial \mathcal{G}}{\partial t} + \mathbf{q}_e \cdot \tilde{\nabla} \mathcal{G} - \frac{q_e}{2 \tilde{\delta}} \left[5.6 \left((c_\tau)_{\text{eq}}^{1/2} - c_\tau^{1/2} \right) \right] - \frac{q_e}{B_{\text{eq}} \delta_1^*} \left[\frac{C_{f1}}{2} - \left(\frac{H-1}{A_{\text{eq}} K_{\text{dl}} H} \right)^2 \right] + \tilde{\nabla} \cdot \mathbf{q}_e = 0 \quad (14)$$

2. Transition

The e^N envelope method is adopted for modeling laminar-to-turbulent flow transition for its simplicity and effectiveness. This method is based on the Orr-Sommerfeld linear flow instability theory, and characterizes natural transition by monitoring the growth of the Tollmien-Schlichting (TS) waves.

Fig. 1 illustrates the notional evolution of flows undergoing transition within a boundary layer. The TS wave fluctuation magnitude q' is defined in Eq. (5), and relates to the small Reynolds stress in the laminar regime. In the standard e^N envelope method, the amplification factor $\tilde{n} \equiv \ln(q'/q'_0)$ is defined as the natural exponent of the amplification ratio, where the initial disturbance level q'_0 is governed by the boundary layer's receptivity to the background flow.

Fig. 1 Laminar-to-turbulent flow transition in a generic boundary layer (top) and the corresponding evolution of the Reynolds velocity fluctuation q' in the natural logarithmic scale (bottom). (Flow transition is assumed to occur instantaneously, whereas the size of the transitional flow region is exaggerated in this figure. Within the transition region, magenta and red curves denote the actual and modeled evolution of q' , respectively.)

Given the relation that $\mathcal{G} = \tilde{n} + \ln(q'_0/q_e)$, the TS wave growth in the laminar flow regime is governed by the following amplification equation in the variable $\mathcal{G}$,

$$\frac{\partial \mathcal{G}}{\partial t} + \mathbf{q}_e \cdot \tilde{\nabla} \mathcal{G} - \frac{q_e}{\theta_{11}} f_N = 0 \quad (15)$$

The growth rate function f_N is given by the following expression,

$$f_N(H; Re_{\theta_{11}}) = R \frac{d\tilde{n}}{dRe_{\theta_{11}}} \theta_{11} \frac{dRe_{\theta_{11}}}{dx} \quad (16)$$

$$\text{where } R = \frac{1}{2} + \frac{1}{2} \tanh \left[10 (\ln Re_{\theta_{11}} - \ln Re_{\theta_{11,0}}) \right] \quad (17)$$

$$\ln Re_{\theta_{11,0}} = \frac{5.738}{(H-1)^{0.43}} + 1.612 \left[\tanh \left(\frac{14}{H-1} - 9.24 \right) + 1 \right] \quad (18)$$

$$\frac{d\tilde{n}}{dRe_{\theta_{11}}} = 0.028(H-1) - 0.0345 \exp \left[- \left(\frac{3.87}{H-1} - 2.52 \right)^2 \right] \quad (19)$$

$$\theta_{11} \frac{dRe_{\theta_{11}}}{dx} = -0.05 + \frac{2.7}{H-1} - \frac{5.5}{(H-1)^2} + \frac{3.0}{(H-1)^3} + 0.1 \exp \left(\frac{-20}{H-1} \right) \quad (20)$$

The correlations (18), (19), and (20) are obtained by fitting the e^N envelope growth rates computed based on the Orr-Sommerfeld equation for self-similar flows [23]. The ramp function R given by the expression (17) is introduced to smoothly model the onset of TS wave growth (i.e. at the first neutrally stable locality); that is, R is effectively zero and one, respectively, before and after the instability onset.

By definition, the initial value of $\tilde{n}$ at a background inflow boundary or a flow stagnation location (where $q_e = 0$) is $\tilde{n}_0 = 0$, and corresponds to the initial disturbance level q'_0 . For unsteady problems, such $\tilde{n}_0$ follows from the initial condition. However, steady-state problems with a vanishing time derivative (i.e. $\partial(\cdot)/\partial t = 0$) require prescribing the initial value $\tilde{n}_0$. In order to avoid explicitly identifying the stagnation location, we enforce the initial condition on $\tilde{n}$ weakly by introducing a source term to the steady-state amplification equation as follows,

$$\mathbf{q}_e \cdot \tilde{\nabla} \mathcal{G} - \frac{q_e}{\theta_{11}} f_N + (1-R) \frac{1}{t_{\text{ref}}} \exp \left(- \frac{q_e^2}{q_{\text{ref}}^2} \right) (\tilde{n} - \tilde{n}_0) = 0 \quad (21)$$

where R is the ramp function defined in Eq. (17), and the reference time and velocity scales are chosen to be $t_{\text{ref}} = \delta^2 \rho_e / \mu_e$ and $q_{\text{ref}} = q_\infty$ respectively. The added source is designed to be nonzero at flow stagnation to impose the initial value of $\tilde{n}$, and to vanish after the instability onset in order not to interfere with the growth of TS waves.

The nonlinear breakdown to transition is assumed to trigger when the amplification factor $\tilde{n}$ reaches some critical threshold $\tilde{n}_{\text{crit}}$ that reflects the background disturbance level. Such a nonlinear breakdown, if any, is assumed to occur so rapidly (over an infinitesimal span) that it effectively delimits laminar and turbulent flows; that is,

$$\tilde{n} < \tilde{n}_{\text{crit}} \rightarrow \text{laminar}, \quad \tilde{n} \geq \tilde{n}_{\text{crit}} \rightarrow \text{turbulent} \quad (22)$$

We note that the transition criterion (22) is solely based on the amplification ratio identified with $\tilde{n}$ (regardless of the absolute magnitude of q'), and, together with Eq. (21), forms a complete transition formulation.

Supposing the initial disturbance level q'_0 is quantifiable, the fluctuation at transition is then given by,

$$q'_{\text{crit}} = q'_0 \exp(\tilde{n}_{\text{crit}}) = Q'_{\text{crit}} q_e, \quad Q'_{\text{crit}} \equiv \frac{q'_0}{q_e} \exp(\tilde{n}_{\text{crit}}) \quad (23)$$

where the critical threshold Q'_{crit} reflects the magnitude of q'_0 . The exact value of Q'_{crit} is elusive in practice [15], and Ref. [12] uses $Q'_{\text{crit}} \approx 0.01$ as a plausible modeling choice. It follows from Eqs. (5) and (23) that,

$$\tilde{n} = \mathcal{G} - \ln Q'_{\text{crit}} + \tilde{n}_{\text{crit}}, \quad c_\tau^{1/2} = \exp \mathcal{G} = Q'_{\text{crit}} \exp(\tilde{n} - \tilde{n}_{\text{crit}}) \quad (24)$$

which relate both $\tilde{n}$ and c_τ to the variable $\mathcal{G}$.

Additionally, in the flow transition process as shown in Fig. 1, the Reynolds velocity fluctuation q' is modeled to change from the critical threshold q'_{crit} that triggers nonlinear breakdown to the initial turbulent value $q'_{\text{T, init}}$. While the value q'_{crit} is determined by specifying Q'_{crit} , the value $q'_{\text{T, init}}$ needs to be chosen to provide an inflow boundary condition for the turbulent flow as in Eq. (28).

The e^N envelope transition formulation discussed in this section also applies to forced transition, with an additional criterion that flow transition can be triggered at a location that is fixed a priori. Bypass and cross-flow transition mechanisms can also be incorporated into the current e^N envelope method as done in MSES [24] and Ref. [12] respectively, despite potential limitations on these modeling choices [15]. They can be handled with the same numerical treatment for transition presented in this paper, and thus are not elaborated.

3. Boundary Conditions

The present IBL equations are hyperbolic, including Eqs. (2), (3), (14), and (21). Thus, they need to be closed with a number of boundary conditions as governed by the characteristics that are approximately aligned with the edge velocity $\mathbf{q}_e$. Various types of boundary conditions for 2D flows are discussed as follows, and can be readily extended to 3D problems in principle.

Inflow: At the inflow boundary, all characteristics enter the flow domain, and hence Dirichlet data need to be prescribed on all the convected quantities $\{\mathbf{p} \cdot \hat{\mathbf{t}}, k, \mathcal{G}\}$. Since the IBL solution assumes specific profile families, alternative integral quantities such as $\hat{\mathbf{e}}_1 \cdot \bar{\bar{\mathbf{P}}} \cdot \hat{\mathbf{t}}$ and $\mathbf{K} \cdot \hat{\mathbf{t}}$ can be prescribed instead of $\mathbf{p} \cdot \hat{\mathbf{t}}$ and k respectively. We note that Eqs. (2) and (3) are derived from mass and momentum conservation laws [1]. Therefore, it is more appropriate to conserve mass (via $\mathbf{M} \cdot \hat{\mathbf{t}}$ for example) in lieu of kinetic energy. Also, a boundary condition on $\mathcal{G}$ is equivalent to that of $\tilde{n}$ and c_τ . Then, the Dirichlet conditions for the inflow boundary become,

$$\mathbf{M} \cdot \hat{\mathbf{t}} = M_{t_{\text{BC}}}, \quad \hat{\mathbf{e}}_1 \cdot \bar{\bar{\mathbf{P}}} \cdot \hat{\mathbf{t}} = P_{1t_{\text{BC}}}, \quad \tilde{n} = \tilde{n}_{\text{BC}} \text{ or } c_\tau = c_{\tau_{\text{BC}}} \quad (25)$$

where specifying $\mathbf{M} \cdot \hat{\mathbf{t}}$ and $\hat{\mathbf{e}}_1 \cdot \bar{\bar{\mathbf{P}}} \cdot \hat{\mathbf{t}}$ is equivalent to prescribing mass and momentum thicknesses (i.e. δ_1^* and θ_{11} respectively) in conventional IBL methods.

Outflow: The outflow boundary are assumed to be the exit of the characteristics, and thus does not require any boundary condition. The current IBL formulation does not consider outflow boundaries of severely separated flows, where the flow and thus the characteristics reverse significantly.

Interface: Interfaces that demarcate viscous flow domains usually arise, for example, at the trailing edge of an airfoil that joins the surface-bound boundary layers and the ensuing wake. Since the characteristics are determined from the flow velocity $\mathbf{q}_e$, the interface conditions are considered as the outflow and inflow boundary conditions for the upstream and downstream domains respectively. The particular form depends on the specific problem and configuration, but the general principle is to enforce conservation laws (mass and momentum) and consistency in the convected quantity $\mathcal{G}$.

4. Summary

The aforementioned IBL equations and boundary conditions are summarized using a canonical example of airfoil-wake configuration as illustrated in Fig. 2. In this example, the physical domain of a 2D IBL formulation (i.e. an open set $\Omega \subset \mathbb{R}^2$) is formed as the union of three open sets: the laminar boundary layer Ω_L^{BL} , the turbulent boundary layer Ω_T^{BL} , and the turbulent wake Ω_T^{wake} . The transition front $\Gamma_{\text{tr}} = \overline{\Omega_L^{\text{BL}}} \cup \overline{\Omega_T^{\text{BL}}}$ defines the interface between laminar and turbulent boundary layers. The trailing edge (TE) $\Gamma_{\text{TE}} = \overline{\Omega_T^{\text{BL}}} \cup \overline{\Omega_T^{\text{wake}}}$ separates the turbulent boundary layer and the wake. The outflow boundary of $\overline{\Omega_T^{\text{wake}}}$ (and Ω) is denoted by Γ_{out} .

Fig. 2 Example IBL physical domain of a 2D airfoil-wake configuration

For the laminar boundary layer, the governing equations are Eqs. (2), (3), and (21) defined on Ω_L^{BL} with laminar boundary layer closures. We note that the variables $\{\delta, \mathcal{A}\}$ at the stagnation location within Ω_L^{BL} is automatically determined by Eqs. (2) and (3), following the same principle as the Falkner-Skan solution with linear edge velocity distribution (i.e. stagnation point flow) [6]. The transition front Γ_{tr} forms an outflow boundary without any boundary condition.

The turbulent boundary layer is governed by Eqs. (2), (3), and (14) defined on Ω_T^{BL} with turbulent boundary layer closures. Inflow boundary conditions are formulated at Γ_{tr} using the following Dirichlet data,

$$\delta_{1\text{BC}}^* = (\delta_1^*)_{\text{L}, \Gamma_{\text{tr}}} \quad (\text{mass conservation}) \quad (26)$$

$$\theta_{11\text{BC}} = (\theta_{11})_{\text{L}, \Gamma_{\text{tr}}} \quad (\text{momentum conservation}) \quad (27)$$

$$c_{\tau\text{BC}} = c_{\tau\text{T}, \text{init}} \quad (\text{initial turbulent shear stress condition}) \quad (28)$$

where the righthand-side terms with the subscript “L, Γ_{tr} ” are obtained from the outflow boundary state of the laminar boundary layer at Γ_{tr} . In Eq. (28), the value $c_{\tau\text{BC}}$ effectively prescribes $q'_{\text{T}, \text{init}}$ at the turbulent onset (as shown in Fig. 1), and $c_{\tau\text{T}, \text{init}}$ can be modeled as follows,

$$c_{\tau\text{T}, \text{init}} = \left[\left(1.8 \exp \left(-\frac{3.3}{H-1} \right) \right)^2 (c_{\tau})_{\text{eq}} \right]_{\text{L}, \Gamma_{\text{tr}}} \quad (\text{XFOIL [22]}) \quad (29)$$

$$\text{or} \quad c_{\tau\text{T}, \text{init}} = c_{\tau\text{crit}} \quad (\text{Ref. [12]}) \quad (30)$$

where Eq. (30) is adopted in the current formulation. The outflow boundary in this case is the trailing edge Γ_{TE} .

The turbulent wake state on Ω_T^{wake} satisfies Eqs. (2), (3), and (14) with turbulent wake closures. Inflow boundary conditions are formulated at Γ_{TE} with the following Dirichlet data (the same as XFOIL and Ref. [1]),

$$(\delta_1^*)_{\text{wake}, \Gamma_{\text{TE}}, \text{BC}} = (\delta_1^*)_{\text{BL}, \Gamma_{\text{TE}}, \text{upper}} + (\delta_1^*)_{\text{BL}, \Gamma_{\text{TE}}, \text{lower}} + h_{\text{TE}} \quad (\text{mass conservation}) \quad (31)$$

$$(\theta_{11})_{\text{wake}, \Gamma_{\text{TE}}, \text{BC}} = (\theta_{11})_{\text{BL}, \Gamma_{\text{TE}}, \text{upper}} + (\theta_{11})_{\text{BL}, \Gamma_{\text{TE}}, \text{lower}} \quad (\text{momentum conservation}) \quad (32)$$

$$(c_{\tau})_{\text{wake}, \Gamma_{\text{TE}}, \text{BC}} = \frac{(\theta_{11} c_{\tau})_{\text{BL}, \Gamma_{\text{TE}}, \text{upper}} + (\theta_{11} c_{\tau})_{\text{BL}, \Gamma_{\text{TE}}, \text{lower}}}{(\theta_{11})_{\text{wake}, \Gamma_{\text{TE}}}} \quad (\text{shear stress consistency}) \quad (33)$$

where $h_{\text{TE}} \geq 0$ is the airfoil trailing edge thickness, and the righthand-side terms with the subscript “BL, Γ_{TE} ” are obtained from the turbulent boundary layer outflow boundary states at the trailing edge Γ_{TE} . The wake outlet Γ_{out} constitutes the outflow boundary, and requires no boundary condition.

The overall viscous formulation comprises individual formulations of all the sub-domains: Ω_L^{BL} , Ω_T^{BL} , and Ω_T^{wake} . It is worth noting that the transition front Γ_{tr} depends on the unknown IBL variables via the transition criterion, and poses a key challenge on the numerical solution.

C. Viscous-Inviscid Interaction

The viscous-inviscid interaction formulation is aimed to allow for flexible and tight coupling. The key components are summarized here, while Ref. [1] gives further details. The unsteady terms (i.e. $\partial(\cdot)/\partial t$) in all the equations are dropped in the subsequent discussion since the current focus is on steady-state flows.

The inviscid formulation can be chosen flexibly, while Eq. (1) is used as an example. The IBL formulation is composed of Eqs. (2), (3) and (21) in laminar regions, and Eqs. (2), (3) and (14) in turbulent regions. The inviscid and viscous flow equations do not interact directly by design. Instead, their coupling is realized by additional auxiliary equations,

$$\Lambda - \tilde{\nabla} \cdot \mathbf{M} = 0 \quad (34)$$

$$\mathbf{q}_e - \mathbf{q}_i = 0 \quad (35)$$

where Λ and $\mathbf{q}_e$ are the auxiliary variables. The mass defect flux $\mathbf{M} = \rho_e \delta_1^* \mathbf{q}_e$ depends on the IBL solution and the auxiliary variable $\mathbf{q}_e$. The inviscid flow velocity $\mathbf{q}_i$ is obtained from the inviscid solution using $\mathbf{q}_i = \nabla \Phi$.

Table 1 summarizes the components of the current viscous-inviscid interaction formulation, while Section IV presents more details about the coupled solution scheme at the level of discrete equations. The inviscid formulation can be swapped flexibly, and strong coupling is achieved by simultaneously solving the inviscid, viscous and auxiliary equations.

Table 1 List of abbreviations, variables, residuals and governing equations in the coupled global system

Abbreviation	Variable Q	Residual $\mathcal{R}$	Governing Equation
IBL	$\delta, \mathcal{A}, \mathcal{G}$	2D IBL	(2), (3), (14) or (21)
inv	Φ	Inviscid	(1)
auxi	Λ	Auxiliary inviscid	(34)
auxv	$\mathbf{q}_e$	Auxiliary viscous	(35)

III. Numerical Discretization

This section introduces the numerical discretization of the aforementioned viscous-inviscid formulation. The inviscid solver uses a panel method that is described with more details in Ref. [1]. The IBL equations are discretized using a DG FEM. The discretization of the auxiliary equations (34) and (35) is chosen to be consistent with that of the viscous and inviscid formulations. These discretizations have been elaborated in Ref. [1], and thus are not elaborated in this paper. The current discussion focuses on the additional numerical treatment within the DG FEM developed for flow transition.

A. Discontinuous Galerkin Formulation

The 2D steady-state IBL equations, (Eqs. (2), (3), (14) and (21) without time-dependent terms) are discretized using the DG FEM for manifold partial differential equations (PDEs) presented in Ref. [1].

The computational domain identified with an open set Ω is discretized into a triangulation $\mathcal{T}_h$ comprised of disjoint open finite elements K such that

$$\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} \overline{K} \quad (36)$$

The DG finite element solution space is

$$\mathcal{V}_h \equiv \{v_h \in L^2(\Omega) : v_h|_K \in \mathcal{P}^p(K), \forall K \in \mathcal{T}_h\} \quad (37)$$

where $\mathcal{P}^p(K)$ denotes the space of polynomials that have a degree up to p and are restricted to the element K . Let $\{\mathcal{W}_j\}$ ($j = 1, 2, \dots$) be a complete set of basis functions of $\mathcal{V}_h$ that are locally supported on finite elements and

discontinuous across element boundaries. The DG approximation of the primary unknowns $\mathbf{v}$ is

$$\mathbf{v}_h|_K(\xi) = \sum_j \mathbf{v}_{h,j} \mathcal{W}_j(\xi) \quad \forall K \in \mathcal{T}_h \quad (38)$$

Similar to the solution discretization, the shape of the triangulation $\mathcal{T}_h$ as defined by the position vector $\mathbf{r}|_K$ is approximated as

$$\mathbf{r}_h|_K(\xi) = \sum_j \mathbf{r}_{h,j} \mathcal{W}_j(\xi) \quad \forall K \in \mathcal{T}_h \quad (39)$$

The local basis vector of an element K is conveniently constructed as a unit vector tangent to the element,

$$\hat{\mathbf{e}} \equiv \frac{\partial \mathbf{r}_h / \partial \xi}{\|\partial \mathbf{r}_h / \partial \xi\|}, \quad \frac{\partial \mathbf{r}_h}{\partial \xi} = \sum_j \mathbf{r}_{h,j} \frac{\partial \mathcal{W}_j}{\partial \xi} \quad (40)$$

which is allowed to be discontinuous across finite element interfaces.

Each of the scalar IBL equations (with the vector Eq. (2) resolved along $\hat{\mathbf{e}}$) is abstracted into a generic form of first-order PDE as follows,

$$\tilde{\nabla} \cdot \mathbf{F}(\mathbf{v}) + S(\mathbf{v}) = 0 \quad (41)$$

Then, the discrete equations in the DG formulation are given as follows,

$$\mathcal{R}_{\text{IBL}}(\mathbf{v}_h, \mathcal{W}) \equiv \sum_{K \in \mathcal{T}_h} \int_K \left(\mathcal{W} S(\mathbf{v}_h) - \tilde{\nabla} \mathcal{W} \cdot \mathbf{F}(\mathbf{v}_h) \right) d\ell + \sum_{\partial K \in \partial \mathcal{T}_h} \mathcal{W} \widehat{\mathbf{t} \cdot \mathbf{F}(\mathbf{v}_h)} = 0, \quad \forall \mathcal{W} \in \mathcal{V}_h \quad (42)$$

where $\partial \mathcal{T}_h$ denotes the set of all the element boundaries ∂K , and the numerical flux $\widehat{\mathbf{t} \cdot \mathbf{F}(\mathbf{v}_h)}$ is defined using a full upwinding or Lax-Friedrichs scheme. The discretization (42) essentially follows the DG FEM presented in Ref. [1], and remains valid if flow transition occurs at a boundary that is known a priori, such as the trailing edge Γ_{TE} , or if there is no flow transition in the computational domain.

The interface conditions (31), (32), and (33) at a trailing edge Γ_{TE} are imposed strongly following the treatment in Ref. [1]. The fluxes at outflow boundaries are evaluated using the finite element solution at the corresponding boundaries.

B. Flow Transition Treatment

As discussed in Section II.B.4, the IBL problem with free transition features a solution-dependent interface (i.e. the transition front Γ_{tr}) within the computational domain. In consequence, two major complications arise. First, the overall IBL formulation in the presence of flow transition involves disparate governing equations (including the underlying closure models) across the transition front, for example, between $\Omega_{\text{L}}^{\text{BL}}$ and $\Omega_{\text{T}}^{\text{BL}}$ of Fig. 2. Additional interface conditions are also introduced at transition, such as Eqs. (26), (27), and (28). Secondly, a free transition location Γ_{tr} depends on the unknown variable $\tilde{n}$ via the transition criterion (22), and is thus unknown prior to the solution of $\tilde{n}$ as wells as other IBL variables.

The free-transition problem belongs to the broad range of physical problems involving stationary or moving interfaces between sub-domains. To solve these problems, various schemes for interface representation and PDE discretization have been developed to date, of which comprehensive reviews can be found in Refs. [25, 26]. One criterion for categorizing these existing methods is their mesh conformity to the interface. Adaptive conformal meshing methods, such as the arbitrary Lagrangian-Eulerian (ALE) approach, are designed to accurately track the interface, but generally suffers from meshing limitations, including high computational cost and intolerance to drastic topological changes. Hence, we are motivated to adopt alternative methods that apply to fixed meshes. These methods are generally constructed by augmenting conventional numerical discretization schemes, e.g. by adding degrees of freedom (DOFs), in order to resolve the interface to certain extent. Such resolution can be distributed/diffuse (e.g. as in the immersed boundary/interface/domain methods) or sharp (e.g. with the enriched FEM). The choice of numerical discretization has a direct bearing on the accuracy, robustness, efficiency, and implementation of the overall numerical solution algorithm.

In view of potential implications of the numerical treatment, and to account for the presence of flow transition in particular, the existing DG discretization of the IBL equations in Section III.A needs to be modified accordingly. To that end, two categories of solution are pursued and compared in this paper: fitted and captured transition. The fitted

transition approach explicitly identifies the topology of the transition front (as if it is fitted, hence the name), and applies potentially different numerical discretization schemes to the respective problems associated with the sub-domains delimited by the interface. In contrast, the captured transition strategy solves the overall IBL problem with a unified numerical discretization, while representing the transition front implicitly based on the transition criterion (22).

Both fitted and captured transition methods solve the same physical problem in the IBL formulation of Section II.B. Their primary distinction lies in the specific numerical treatment of the governing equations and interface conditions.

C. Fitted Transition

The fitted transition approach is presented in this section. Existing examples of fitted transition treatment include MSES and XFOIL in the 2D and finite difference setting. These examples explicitly track the flow transition by marching the solution of the TS wave amplification equation in the streamwise direction. The dependence of the transition location on the IBL unknowns is assimilated into the nonlinear system of IBL equations, which, coupled with the inviscid formulation, are solved using an under-relaxed global Newton method. The under-relaxation also leverages space marching for solution re-conditioning between nonlinear solution iterations, but is largely specific to the 2D finite difference scheme in use. In addition, mass and momentum conservation at the transition front is satisfied automatically by judiciously choosing the mass and momentum defect thicknesses (i.e. δ_1^*, θ_{11} respectively) as working variables, which are assumed to be continuous in the finite difference discretization. However, that specific choice of primary unknowns differs from the current profile family definition [1]. Also, the space marching algorithm is not readily transferable to the current DG IBL formulation and general 3D configurations.

Numerical methods with sharp interface representation also exist in other contexts. Notable examples in the finite difference setting include Refs. [25, 27]. Conventional FEM have also been “enriched” in various ways to handle sharp interfaces, for example, in Refs. [28–34]. However, the aforementioned examples either assume the interface to be solution-independent, or relax the coupling between the equation solution and the interface identification using iterative schemes.

In the current work, the IBL solution and the transition front identification are carried out simultaneously in order to maintain strong coupling, and a cut-cell treatment is formulated to enable fitted transition within the DG FEM. We start by distinguishing the IBL equations and primary unknowns that are defined in the laminar, turbulent or both regions. Let the computational domain Ω be decomposed into laminar and turbulent regions (i.e. Ω_L and Ω_T respectively), such that the closure of Ω is the union of the closures of Ω_L and Ω_T (i.e. $\bar{\Omega} = \bar{\Omega}_L \cup \bar{\Omega}_T$), and the transition front is $\Gamma_{tr} = \bar{\Omega}_L \cap \bar{\Omega}_T$. Here and subsequently, the subscripts “L” and “T” stand for laminar and turbulent respectively. The overall formulation in a generic form is summarized as follows

$$\tilde{\nabla} \cdot \mathbf{F}(\mathbf{v}) + S(\mathbf{v}) = 0 \quad \text{in } \Omega \quad (43)$$

$$\tilde{\nabla} \cdot \mathbf{F}_L(\mathbf{v}_L) + S_L(\mathbf{v}_L) = 0 \quad \text{in } \Omega_L \quad (44)$$

$$\tilde{\nabla} \cdot \mathbf{F}_T(\mathbf{v}_T) + S_T(\mathbf{v}_T) = 0 \quad \text{in } \Omega_T \quad (45)$$

Table 2 categorizes the IBL equations and primary unknowns according to the generic form. We note that the variable $\mathcal{G}$ is defined separately for Eqs. (14) and (21) in the current fitted transition method. The six IBL equations in Table 2 are discretized differently depending on their corresponding generic form.

Table 2 IBL equations and unknowns categorized based on their domain of definition

Generic Form	Primary Unknown	Governing Equation
(43)	$\mathcal{G}$	(21)
(44)	$\delta_L, \mathcal{A}_L$	(2), (3) with laminar closures
(45)	$\delta_T, \mathcal{A}_T, \mathcal{G}$	(2), (3), (14) with turbulent closures

In the current formulation, the transition front Γ_{tr} is approximated with the level set $\tilde{n} = \tilde{n}_{crit}$ of the linear interpolant of the nodal values $\tilde{n}$. The resulting topology of the transition front Γ_{tr} is affine on a given finite element, and is a function of the variable $\tilde{n}$. Curved transition front approximation in 3D configurations remains to be examined in the future.

A cut-cell treatment is applied to each finite element K_{tr} that is divided by Γ_{tr} into two sub-elements: K_L (laminar) and K_T (turbulent); that is,

$$\bar{K}_{\text{tr}} = \bar{K}_L \cup \bar{K}_T, \quad K_L \cap K_T = \emptyset, \quad \Gamma_{\text{tr},K} \equiv \bar{K}_L \cap \bar{K}_T \subset \Gamma_{\text{tr}} \quad (46)$$

where $\Gamma_{\text{tr},K}$ denotes the segment of the transition front on the element $\bar{K}_{\text{tr}}$. This cut-cell configuration is illustrated in Fig. 3, along with additional basis functions defined on the sub-elements.

Fig. 3 Division of a transitional element K_{tr} into laminar and turbulent sub-elements K_L and K_T with locally supported basis functions $\mathcal{W}_L$ and $\mathcal{W}_T$ respectively (The linear Lagrange basis is shown as an example)

The generic form (43) is discretized using the plain DG discretization (42) with the original approximate solution space $\mathcal{V}_h$. In order to track the transition front based on the local solution $\tilde{n}$ (e.g. at individual finite elements and their interfaces) without space marching, the TS wave amplification equation is extended from the laminar region to the entire computational domain, by defining the source term S of Eq. (21) in the turbulent region Ω_T as,

$$S = \begin{cases} S_{\Gamma_{\text{tr},K}} & \text{on } K_T \subset K_{\text{tr}} \\ S_T & \text{on } K \subset \Omega_T \end{cases} \quad (47)$$

where the turbulent sub-element K_T , the transitional element K_{tr} , and the transition segment $\Gamma_{\text{tr},K}$ are defined in (46) and illustrated in Fig. 3. The source term $S_{\Gamma_{\text{tr},K}}$ is evaluated at $\Gamma_{\text{tr},K}$, and interpolated over K_T . Both the evaluation and interpolation are local to the finite element K_{tr} . The value of S_T is chosen to be constant and negative to ensure the growth $\tilde{n}$ in the fully turbulent elements and avoid fictitious re-laminarization. The extension of the amplification equation is justified by the fact that the growth of $\tilde{n}$ remains largely unaltered in the laminar region and the vicinity of the transition front.

Next, for the generic form (44), the original DG discretization (42) still applies to the set of finite elements K that are in the interior of the laminar region Ω_L (i.e. $K \in \mathcal{T}_h$ and $K \subset \Omega_L$). Modification is introduced to those elements whose closure intersects the transition front Γ_{tr} . The original DG elemental residual equation associated with the element K_{tr} is replaced with the discretization on the sub-element K_L ; that is, $\forall \mathcal{W}_L \in \mathcal{P}^p(K_L)$,

$$0 = \sum_{\Gamma_{\text{tr},K}} \mathcal{W}_L \hat{\mathbf{t}} \cdot \mathbf{F}_L(\mathbf{v}_{L,h}) + \sum_{\partial K_L \setminus \Gamma_{\text{tr},K}} \mathcal{W}_L \mathbf{t} \cdot \widehat{\mathbf{F}_L(\mathbf{v}_{L,h})} + \int_{K_L} \left(\mathcal{W}_L S_L(\mathbf{v}_{L,h}) - \tilde{\nabla} \mathcal{W}_L \cdot \mathbf{F}_L(\mathbf{v}_{L,h}) \right) d\ell \quad (48)$$

where the weighting function $\mathcal{W}_L$ is compactly supported on the sub-element K_L , and replaces its original counterpart $\mathcal{W}$ that is supported on K_{tr} , as illustrated in Fig. 3.

In order for the discrete equations to be well-conditioned, the solution approximation (38) on the element K_{tr} is also modified to use the same basis function $\mathcal{W}_L$,

$$\mathbf{v}_{L,h}|_{K_L}(\xi) = \sum_j \mathbf{v}_{L,h,j} \mathcal{W}_{L,j}(\xi) \quad (49)$$

Assuming a laminar-to-turbulent transition, the boundary $\Gamma_{\text{tr},K}$ corresponds to the laminar outflow. Thus, the plain DG treatment of the outflow boundary applies.

Another complication is that the number of DOFs in the finite element approximation $\mathbf{v}_{L,h}$ depends on the location of the transition front, which itself is solution-dependent. Since the dynamical management of the DOF count (i.e. in a solution-dependent manner) is cumbersome from an implementation perspective, the solution approximation $\mathbf{v}_{L,h}$ is statically enriched with redundant DOFs defined on the turbulent elements as follows,

$$\mathbf{v}_{L,h}|_K(\xi) = \sum_j \mathbf{v}_{L,h,j} \mathcal{W}_j(\xi) \quad \forall K \in \mathcal{T}_h \text{ and } K \subset \Omega_T; \mathcal{W}_j \in \mathcal{P}^p(K) \quad (50)$$

and closed with additional dummy equations (which are independent of the DG discrete equations). In doing so, the total number of DOFs is maintained constant. However, the residual equation associated with each weighting function $\mathcal{W}_j$ (or $\mathcal{W}_{L,j}$) is allowed to change dynamically between the dummy, plain DG, and cut-cell DG forms. This poses a challenge on the nonlinear solution method and is addressed in Section IV.B.

The same quadrature rule (e.g. Gauss-Legendre quadrature) can be used for evaluating the elemental (line) integrals in Eqs. (42) and (48) except for different domains of integration (i.e. K versus K_L respectively). Such convenience is generally not available in three-dimensional (3D) cases where the elements K and K_L can assume different topologies (e.g. triangle versus quadrilateral). In those cases, the quadrature rule for integration over the sub-element K_L needs to be modified with extra implementation efforts.

Finally, the discretization of the generic form (45) is also modified with a similar cut-cell treatment on the elements K_{tr} intersecting the transition front; that is, $\forall \mathcal{W}_T \in \mathcal{P}^p(K_T)$,

$$0 = \sum_{\Gamma_{tr,K}} \mathcal{W}_T F_{tr,K} + \sum_{\partial K_T \setminus \Gamma_{tr,K}} \mathcal{W}_T \mathbf{t} \cdot \overline{\mathbf{F}_T(\mathbf{v}_{T,h})} + \int_{K_T} \left(\mathcal{W}_T S_T(\mathbf{v}_{T,h}) - \tilde{\nabla} \mathcal{W}_T \cdot \mathbf{F}_T(\mathbf{v}_{T,h}) \right) d\ell \quad (51)$$

where the basis function $\mathcal{W}_T$ is compactly supported on the turbulent sub-element K_T , and the solution approximation is modified similarly to the cut-cell treatment of the generic form (44). A free (flux) variable $F_{tr,K}$ is introduced on each finite element for each scalar equation. In effect, that variable serves as a Lagrange multiplier to facilitate the strong imposition of the inflow boundary conditions (26), (27), and (28) on $\Gamma_{tr,K}$. On elements that do not intersect the transition front, the free variable $F_{tr,K}$ becomes redundant, and is closed with a dummy equation accordingly.

D. Captured Transition

As an alternative to the fitted transition treatment in Section III.B, a captured transition approach is presented to eliminate the need of explicit tracking the transition front and fit with the plain DG discretization.

We consider a unified set of IBL primary unknowns $\mathbf{v} = \{\delta, \mathcal{A}, \mathcal{G}\}$ defined on the entire computational domain Ω . The IBL equations defined on individual sub-domains (e.g. those summarized in Section II.B.4) can be cast into the generic form (41) defined throughout Ω . Then, the task becomes to define the flux $\mathbf{F}$ and the source S for each equation in a unified manner.

First, for the momentum and kinetic energy equations, i.e. (2) and (3) respectively, the fluxes and sources are defined as follows,

$$\mathbf{F} = \begin{cases} \overline{\mathbf{P}}_L & \text{on } \Omega_L \\ \overline{\mathbf{P}}_T & \text{on } \Omega_T \end{cases}, \quad S = \begin{cases} \left((\tilde{\nabla} \mathbf{q}_e) \cdot \mathbf{M} - \tau_w \right)_L & \text{on } \Omega_L \\ \left((\tilde{\nabla} \mathbf{q}_e) \cdot \mathbf{M} - \tau_w \right)_T & \text{on } \Omega_T \end{cases} \quad (\text{momentum equation}) \quad (52)$$

$$\mathbf{F} = \begin{cases} \mathbf{K}_L & \text{on } \Omega_L \\ \mathbf{K}_T & \text{on } \Omega_T \end{cases}, \quad S = \begin{cases} \left(\mathbf{D} \cdot \tilde{\nabla} (q_e^2) - 2 \mathcal{D} \right)_L & \text{on } \Omega_L \\ \left(\mathbf{D} \cdot \tilde{\nabla} (q_e^2) - 2 \mathcal{D} \right)_T & \text{on } \Omega_T \end{cases} \quad (\text{kinetic energy equation}) \quad (53)$$

where the subscripts “L” and “T” imply the use of laminar and turbulent closure models respectively. The momentum defect and kinetic energy defect fluxes are conserved at the transition front with $\mathbf{F}_L(\mathbf{v}|_{\Gamma_{tr}}) = \mathbf{F}_T(\mathbf{v}|_{\Gamma_{tr}})$, which is accepted as a plausible relaxation of the interface conditions of mass and momentum conservation discussed in II.B.3.

Then, the amplification equation (21) and the lag equation (14) are combined to define the following flux and source,

$$\mathbf{F} = \mathcal{G} \mathbf{q}_e \text{ on } \Omega, \quad S = \begin{cases} -\mathcal{G} \tilde{\nabla} \cdot \mathbf{q}_e - \frac{q_e}{\theta_{11}} f_N + (1-R) \frac{1}{t_{ref}} \exp\left(-\frac{q_e^2}{q_{ref}^2}\right) (\tilde{n} - \tilde{n}_0) & \text{on } \Omega_L \\ (1-\mathcal{G}) \tilde{\nabla} \cdot \mathbf{q}_e - \frac{q_e}{2\delta} \left[5.6 \left((c_\tau)_{eq}^{1/2} - c_\tau^{1/2} \right) \right] - \frac{q_e}{B_{eq} \delta_1^*} \left[\frac{G_f}{2} - \left(\frac{H-1}{A_{eq} K_{dl} H} \right)^2 \right] & \text{on } \Omega_T \end{cases} \quad (54)$$

At the transition front Γ_{tr} , the variable $\mathcal{G}$ is continuous as a result of the interface condition (30). Alternatively, the formulation (29) can also be used by, for example, introducing an appropriate point source at the transition front, but it presents an inessential modeling difference and thus is not considered in this paper.

The IBL equations have so far been unified into the generic form (41) with primary unknowns $\{\delta, \mathcal{A}, \mathcal{G}\}$. The laminar and turbulent regimes are determined by the value of $\tilde{n}$ based on the transition criterion (22) without explicit tracking the transition front. Hence, the plain DG discretization (42) is directly applicable, which greatly simplifies the required numerical implementation compared to the fitted transition formulation.

We also note that the source terms defined in the formulas (52), (53) and (54) are generally discontinuous across the transition front. Hence, they can lead to the Gibbs phenomenon (with oscillatory solutions) for higher-than-first-order solution approximation (i.e. $p \geq 1$ for the DG solution space (37)). This issue can potentially be addressed by introducing additional numerical stabilization or adopting a distributed interface representation (e.g. as in Refs. [35–37]). Instead of making these extra modeling choices, this paper focuses on the basic form of captured transition to highlight its convenient implementation and to identify areas of improvement.

IV. Strongly-coupled Solution Procedure

The global discrete system of equations, including the inviscid, viscous and auxiliary equations, are solved simultaneously to achieve strong viscous-inviscid coupling, which has proven to be integral to the solution robustness [2]. The coupled nonlinear system of equations is written compactly as

$$\mathcal{R}(\mathcal{Q}) = \mathbf{0}, \quad \mathcal{R} \equiv \begin{pmatrix} \mathcal{R}_{auxv}(\mathcal{Q}_{auxv}, \mathcal{Q}_{inv}) \\ \mathcal{R}_{auxi}(\mathcal{Q}_{auxv}, \mathcal{Q}_{auxi}, \mathcal{Q}_{IBL}) \\ \mathcal{R}_{IBL}(\mathcal{Q}_{auxv}, \mathcal{Q}_{IBL}) \\ \mathcal{R}_{inv}(\mathcal{Q}_{auxi}, \mathcal{Q}_{inv}) \end{pmatrix}, \quad \mathcal{Q} \equiv \begin{pmatrix} \mathcal{Q}_{auxv} \\ \mathcal{Q}_{auxi} \\ \mathcal{Q}_{IBL} \\ \mathcal{Q}_{inv} \end{pmatrix} \quad (55)$$

where $\mathcal{R}$ and $\mathcal{Q}$ denote the global residual and solution respectively, and their components are summarized in Table 1.

A Newton method is employed to solve the generally nonlinear global system. In the Newton iteration n , the solution is updated via the following formula,

$$\mathcal{R}(\mathcal{Q}^n) + \left[\frac{\partial \mathcal{R}}{\partial \mathcal{Q}} \right]^n \Delta \mathcal{Q}^n = \mathbf{0} \quad (56)$$

$$\mathcal{Q}^{n+1} = \mathcal{Q}^n + \Delta \mathcal{Q}^n \quad (57)$$

The linear system (56) is solved for the solution update $\Delta \mathcal{Q}$. The size of a typical 2D problem is computationally tractable for a direct linear solver in general (e.g. the LU factorization algorithm with partial column pivoting available in the UMFPACK library [38]). An initial solution guess $\mathcal{Q}^0$ is required for the Newton update to start with, for which Ref. [1] provides a heuristic recipe.

Depending on the characteristics of the inviscid solver, the global jacobian can be permuted to optimize fill-in and matrix storage. The present IBL/panel coupling implementation in particular has the following structure,

$$\left[\frac{\partial \mathcal{R}}{\partial \mathcal{Q}} \right] = \begin{pmatrix} \left[\frac{\partial \mathcal{R}_{auxv}}{\partial \mathcal{Q}_{auxv}} \right] & 0 & 0 & \left[\frac{\partial \mathcal{R}_{auxv}}{\partial \mathcal{Q}_{inv}} \right] \\ \left[\frac{\partial \mathcal{R}_{auxi}}{\partial \mathcal{Q}_{auxv}} \right] & \left[\frac{\partial \mathcal{R}_{auxi}}{\partial \mathcal{Q}_{auxi}} \right] & \left[\frac{\partial \mathcal{R}_{auxi}}{\partial \mathcal{Q}_{IBL}} \right] & 0 \\ \left[\frac{\partial \mathcal{R}_{IBL}}{\partial \mathcal{Q}_{auxv}} \right] & 0 & \left[\frac{\partial \mathcal{R}_{IBL}}{\partial \mathcal{Q}_{IBL}} \right] & 0 \\ 0 & \left[\frac{\partial \mathcal{R}_{inv}}{\partial \mathcal{Q}_{auxi}} \right] & 0 & \left[\frac{\partial \mathcal{R}_{inv}}{\partial \mathcal{Q}_{inv}} \right] \end{pmatrix} \quad (58)$$

By the design of the viscous-inviscid formulation, the matrix blocks $\partial \mathcal{R}_{inv} / \partial \mathcal{Q}_{IBL}$ and $\partial \mathcal{R}_{IBL} / \partial \mathcal{Q}_{inv}$ are invariably zero, resulting in the block-diagonal 2-by-2 system on the lower right of the current global jacobian. This prevents direct interdependence between the IBL and inviscid solvers, and thus allows for a flexible choice of the inviscid solver.

For viscous and inviscid solvers that are developed separately, the computation of individual residuals (e.g. $\mathcal{R}_{\text{IBL}}, \mathcal{R}_{\text{inv}}$) is reusable. Adding the auxiliary equations to build the coupled system of equations does not require excessive overhead. The global jacobian is conveniently constructed using the automatic differentiation toolbox developed in an in-house code suite [39].

A. Line Search

In order to enhance the robustness of the nonlinear solver, the aforementioned plain Newton method is augmented with a line-search algorithm. The corresponding solution update formula then becomes

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n + \beta \Delta \mathbf{Q}^n \quad (59)$$

where $\beta > 0$ is a step-sizing factor that shrinks from one by half iteratively in order to limit the solution update in the following situations.

- 1) Residual reduction failure: Any component of the global residual $\mathcal{R}$ fails to decrease, before the solution converges below the prescribed tolerance. A useful relaxation is to allow the residual to grow moderately. It is observed that the initial transient residual growth in some cases helps accelerate subsequent convergence.
- 2) Physical validity failure: the boundary layer thickness parameter δ and the shear stress coefficient c_τ fail to remain strictly positive.

The unlimited case of $\beta = 1$ recovers the the plain Newton solution update in Eq. (57).

The line-search algorithm allows the nonlinear solution update to continue in some solution iterations that would fail otherwise. The resulting nonlinear solution has been observed to be more robust in terms of admitting various initial solution guesses.

B. Under-relaxation

The effectiveness of the Newton method as well as the line-search algorithm is contingent on the smoothness of the residual. However, the equation residuals defined in the fitted transition formulation of Section III.B loses continuity when the transition front moves across finite elements and thus changes the definition of individual residuals (e.g. between a discrete IBL equation and a dummy equation). For example, in the Newton method, the variables $\mathbf{Q}^n$ and $\mathbf{Q}^{n+1}$ (at iteration n) potentially correspond to different transition locations and hence disparate cut-cell configurations. In these situations, definitions of the residuals $\mathcal{R}^n$ and $\mathcal{R}^{n+1}$ are not equivalent. Such discontinuity in the residual with respect to the solution variable poses difficulty to the plain Newton method as well as the line-search algorithm.

On the other hand, if the transition location is assumed to be fixed (e.g. in forced-transition problems), the residual smoothness is maintained, for which the line-search Newton method performs well. Therefore, to improve the robustness in solving free-transition problems using the fitted transition method, we propose a two-layer nonlinear solution scheme as listed in Algorithm 1.

Algorithm 1: Two-layer Newton solution method for free-transition problems

Initialize: Initial solution guess $\mathbf{Q}^0$, relaxation factor $\alpha < 1$, Newton iteration $n = 0$, maximum iteration n_{max}

while Solution $\mathbf{Q}^n$ is not converged and $n \leq n_{\text{max}}$ **do**

Solve Eq. (56) of the free-transition problem for $\Delta \mathbf{Q}^n$

Under-relax the plain Newton solution update (57): $\mathbf{Q}^{n+1} = \mathbf{Q}^n + \alpha \Delta \mathbf{Q}^n$

if Solution $\mathbf{Q}^{n+1}$ converges **then**

Terminate

else

Identify the transition front Γ_{tr}^{n+1} based on $\mathbf{Q}^{n+1}$

Solve the forced transition problem with transition fixed at Γ_{tr}^{n+1} using the line-search Newton method and the initial solution guess $\mathbf{Q}^{n+1}$

Re-conditioning: Assign the forced-transition solution to $\mathbf{Q}^{n+1}$

end

Increment n by 1

end

The outer layer is an under-relaxed Newton method for the free-transition problem. The relaxation factor α is chosen to limit the updated solution from breaching physical validity. The nested layer is the solution of a forced-transition

problem using the line-search Newton method, and serves to “re-condition” the updated solution of each outer Newton iteration. The combination of under-relaxation and re-conditioning alleviates the residual discontinuity issue associated with the solution-dependent cut-cell treatment

V. Results

Numerical experiments are carried out with a focus to verify and compare the numerical discretization schemes for the IBL formulation: both the fitted and the captured transition method. In the test case, a steady-state incompressible flow over the NACA 0004 airfoil (with a finite-thickness trailing edge) is considered. A sample grid configuration is illustrated in Fig. 4. Flow conditions include a zero angle of attack and Reynolds number $Re = 10^5$ (based on the chord).

Fig. 4 Sample grid for NACA 0004 airfoil (64 and 14 elements on the airfoil and the wake respectively)

The DG FEM discretization of the IBL equations uses a polynomial degree $p = 1$, since it is coupled with a linear-vorticity panel method [1]. Accordingly, a three-point Gauss-Legendre quadrature is used for evaluating line integrals in the DG weighted residuals such as those in Eq. (42).

For comparison, XFOIL results are also obtained on the same test case. The IBL method of this paper differs from XFOIL primarily in the closure models (including profile families and the empirically fitted TS wave amplification rate (16)). To minimize the difference, XFOIL is modified to use the interface condition Eq. (30) instead of its default formulation of Eq. (29). Although the IBL method presented in this paper is not expected to produce exactly the same solution as XFOIL, it is still fair to compare characteristics of the numerical discretization, such as the order of accuracy, which are independent of the differences in the closure models.

A. Grid Convergence

A grid refinement study is conducted to investigate the order of accuracy of both the fitted and captured transition methods, in comparison with XFOIL. Each IBL method under consideration is run over the same sequence of quasi-uniformly refined grids. The critical amplification factor is chosen as $\tilde{n}_{crit} = 0.6$, which triggers natural flow transition on the airfoil surface.

The convergence of the sectional drag coefficient c_d is first examined, which is computed from the IBL solution using the Squire-Young method as noted in Ref. [6]. The reference value $(c_d)_{ref}$ of each IBL method is chosen to be the c_d value computed based on the respective solution of the finest grid (with 2,048 elements on the airfoil surface).

The variation of c_d with grid refinement is shown in Figs. 5 and 6. Results of both the fitted transition method and XFOIL demonstrate an asymptotic convergence of c_d with mesh refinement, with an approximately second-order accuracy. This order of accuracy is acceptable since it is no less than that of the respective inviscid or viscous solver (i.e. the panel method or the IBL method respectively).

On the other hand, the captured transition method does not produce a convincingly grid-converged solution in this study. The oscillatory variation of c_d with mesh refinement (i.e. a Gibbs phenomenon) indicates the impact of the numerical discontinuity due to the laminar-to-turbulent closure switch at transition, as mentioned in Section III.D. To address the loss of grid convergence, additional numerical treatment of the discontinuity is necessary. Potential fixes are mentioned in Section III.D and will be investigated in future work.

The convergence of the predicted free transition location is also investigated. Since the test case is a symmetric airfoil at zero angle of attack, the transition locations on the upper and lower surfaces coincide in terms of the chord-wise coordinate, denoted as x_{tr} . The reference transition location $x_{tr,ref}$ of each IBL method is chosen to be the value based on its corresponding solution for the finest grid (with 2,048 elements on the airfoil surface). As illustrated in Fig. 7, the transition location x_{tr} of the fitted transition method and XFOIL also converge asymptotically with mesh refinement and at a second-order accuracy. In comparison, the resulting x_{tr} values of the captured transition approach lack consistent grid convergence.

Fig. 5 Convergence of sectional drag coefficient c_d for various IBL methods

B. Parameter Sensitivity

For the purpose of verification, the sensitivity of the numerical solution with respect to other problem parameters is also studied. The critical amplification factor $\tilde{n}_{\text{crit}}$ is examined in particular since it directly governs the free transition location. It is necessary that the output of interest such as c_d varies continuously with the parameter $\tilde{n}_{\text{crit}}$; otherwise, the output c_d prediction can be ambiguous for the same $\tilde{n}_{\text{crit}}$.

Both the fitted and captured transition methods are run over a sequence of $\tilde{n}_{\text{crit}}$ values on the same grid of 64 elements on the airfoil surface. XFOIL solution is also obtained for the same $\tilde{n}_{\text{crit}}$ sequence, albeit using 96 elements on airfoil surface (since XFOIL cannot produce results robustly on the same 64-element grid). All the $\tilde{n}_{\text{crit}}$ values in this test result in natural transition occurring on the airfoil surface. The variation of the resulting output c_d with the parameter $\tilde{n}_{\text{crit}}$ is illustrated in Fig. 8. The fitted transition and XFOIL results demonstrate a continuous dependence of c_d on $\tilde{n}_{\text{crit}}$, even when the transition front moves across elements of the grid. Such continuity is a desirable characteristic of the numerical discretization.

In comparison, the captured transition results reveal the discontinuity in the current formulation, such as the source term S in Eq. (54) that is discontinuous across the transition front. In consequence, the output c_d of the captured transition method varies discretely when the transition front crosses grid elements or numerical quadrature points within an element, as shown in Fig. 8. In this test case, the captured transition uses a 20-point Gauss-Legendre quadrature rule in order to resolve the discontinuity as transition moves within an element. In comparison, the fitted transition still uses the default 3-point quadrature rule. The issue of discrete c_d - $\tilde{n}_{\text{crit}}$ relation reiterates the need of additional numerical treatment of the discontinuity in the captured transition formulation.

C. Sample IBL Solutions

This section presents instances of the IBL solution for both cases of forced and free transition. In the forced-transition case, the transition is triggered at a fixed location identified with the chord-wise coordinate $x_{\text{tr}} = 0.8c$. Both the fitted transition method and XFOIL are run on the same grid of 128 elements. The captured transition method is not examined in this case since its current form cannot explicitly impose the same turbulent inflow condition (28) at a forced-transition front. As illustrated in Figs. 9 to 11, results of both the fitted transition method and XFOIL match reasonably well, while their differences in the forced-transition case are mainly caused by different choices of closure models.

In the free-transition case, the parameter $\tilde{n}_{\text{crit}} = 0.6$ is used to trigger natural transition on the airfoil surface. Figs. 12 to 14 illustrate results of the fitted and captured transition methods as well as XFOIL. In particular, the amplification factor $\tilde{n}$ growth in Fig. 12 demonstrates the difference in the transition treatment. That is, the $\tilde{n}$ value is defined only in the laminar region in XFOIL, but is defined in the entire boundary layer in both the fitted and the

Fig. 6 Convergence of sectional drag coefficient c_d for individual IBL methods

Fig. 7 Convergence of transition location x_{tr} for various IBL methods

Fig. 8 Variation of sectional drag coefficient c_d with parameter $\tilde{n}_{crit}$

captured transition method. As shown in Fig. 12, the transition locations predicted by the fitted and captured transition methods differ from that of XFOIL, mainly because this paper uses a different growth rate correlation compared to XFOIL. Despite that difference, their results agree qualitatively.

Fig. 9 Forced transition: shear stress coefficient c_τ and normalized edge speed distribution $|q_e/q_\infty|$

Fig. 10 Forced transition: mass defect thicknesses δ_1^* and momentum defect thickness θ_{11}

Fig. 11 Forced transition: skin-friction coefficient C_{f1} (only on airfoil surface) and dissipation coefficient C_D

Fig. 12 Free transition: amplification factor $\tilde{n}$ evolution ($\tilde{n}_{\text{crit}} = 0.6$; only on airfoil surface) and normalized edge speed distribution $|q_e/q_\infty|$

Fig. 13 Free transition: mass defect thicknesses δ_1^* and momentum defect thickness θ_{11}

Fig. 14 Free transition: skin-friction coefficient C_{f1} (only on airfoil surface) and dissipation coefficient C_D

VI. Conclusions

This paper presents numerical discretization schemes that enable free-transition modeling for a strongly-coupled IBL method in the DG FEM setting. Both a fitted and a captured transition approach are developed and compared. The fitted transition method is based on a solution-dependent cut-cell treatment that preserves a sharp representation of the transition front. Numerical results of that method demonstrate numerical characteristics comparable to XFOIL in terms of a second-order accuracy and continuous solution-parameter dependence (i.e. $c_d\text{-}\tilde{n}_{\text{crit}}$). The use of a two-layer Newton method accounts for residual discontinuity associated with the free transition, and contributes to the nonlinear solution robustness. On the other hand, the captured transition approach adopts a plain DG discretization scheme, which significantly simplifies the numerical implementation. However, the test case reveals the issue of numerical discontinuity associated with the straightforward captured transition formulation. This problem indicates a need for additional numerical regularization in order to attain justifiable effectiveness in aerodynamics analysis with free transition.

In future work, both the fitted and the captured transition methods will be extended to 3D configurations. In a 3D case, the captured transition formulation offers more advantageous implementation convenience compared to the fitted transition approach, but requires appropriate treatment of the numerical discontinuity to achieve acceptable reliability. Trade-offs between the two methods will be further examined on 3D IBL problems. In addition, the current closure models, especially the profile families, used in the IBL formulation remain to be improved, in order to robustly accommodate more demanding aerodynamic flow cases. Examples include flows with intense separation bubbles where the transition prediction is very sensitive to the boundary layer solution.

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