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A Mathematically Exact and Well-Determined System of Equations to Close Reynolds-Averaged Navier–Stokes Equations

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Abstract: Since Sir Osborne Reynolds presented the Reynolds-averaged Navier–Stokes (RANS) equations in 1895, the construction of complete closure for RANS equations has been regarded as extremely challenging. Taking into account that the Navier–Stokes equations are not coherent for instantaneous and mean flows, a body of knowledge outside the scope of classical mechanics may be amenable to the closure problem. In this regard, the methodology of physics-to-geometry transformation, which is coherent for both flows, is applied to RANS equations to construct six additional equations. The proposed equations stand out from existing RANS closure models and turbulence quantity transport equations in two respects: they are mathematically exact and well-determined.

Keywords: turbulence modeling; RANS clsoure; physics-to-geometry transformation

MSC: 76F55; 53A05; 53A25

1. Introduction

Since the Reynolds-averaged Navier–Stokes (RANS) equations were first introduced [1], constructing a complete closure for them has remained an open problem. Causal relations over time between mean momenta and stresses in turbulent flow are not generally describable in terms of Navier–Stokes equations, so these are not coherent for instantaneous and mean flows:

$$\mathcal{N}(.) \neq \mathcal{N}(\langle . \rangle), \tag{1}$$

where $\mathcal{N}$ is the Navier–Stokes operator and $\langle . \rangle$ denotes a time- or ensemble-averaging operator. This suggests that mean flow is fundamentally different from instantaneous flow in the scope of classical mechanics, which is a plausible reason why the physical concepts and laws established for instantaneous flows cannot directly apply to mean flows. The notorious difficulty of the closure problem may originate from this difference.

Mathematical approaches make it possible to understand mean flows via instantaneous flow physics, despite the above-described incoherence. For linear flow quantities and operators, the numerical equality derived by the use of the Reynolds decomposition and the fundamental properties of Reynolds-averaging allows for mathematical mimics; examples of this include the mean rate of strain and rotation tensors. For nonlinear ones, such a mimic is not possible since additional terms that require physical analysis arise from the process of Reynolds averaging. In particular, for mathematical approaches to construct a RANS closure, such an appearance of additional unclosed terms is definitely an obstacle even though numerical equality is obtainable. On the other hand, it is also not easy to mathematically derive an exact relation between the Reynolds stress tensor and mean flow quantities without additional unclosed terms. This is a common dilemma encountered whilst constructing a RANS closure.

Modeling has been widely adopted as an alternative methodology since it allows for an explicit formulation of Reynolds stress tensor and is therefore tractable for numerical simulation. However, it resorts to approaches in which mathematical exactness is not

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ensured a priori, such as physical intuition and empiricism, which inevitably lead to the issue of universality. Examples include the linear stress–strain relation with the eddy-viscosity, which was generalized from the Boussinesq hypothesis [2], and the mixing length theory [3]. In particular, for the former, the isotropy eddy-viscosity assumption has represented a key concept for constructing RANS closure models, but its scope of application is limited; it is strictly correct under the condition of $\tau \ll S$, where τ is the turbulent time scale and S is the mean shear time scale [4], while otherwise the linear relation between the Reynolds stress tensor and the mean rate-of-strain tensor is violated in anisotropic turbulent flows (see, e.g., Ref. [5]). Correspondingly, the following efforts were focused on the development of a RANS closure model to obtain high predictive capability for anisotropic turbulent flows. Actually, advanced RANS closure models were devised by incorporating anisotropy into an eddy-viscosity form or considering higher-order stress–strain relations; examples of this include quadratic [6] and cubic $k - \epsilon$ models [7], V2F model [8], and quadratic constitutive relation-based models [9,10]. Recently, it was demonstrated that the above-described shortcoming of linear eddy-viscosity models can be remedied by adopting data processing techniques into existing RANS closure models (see, e.g., Refs. [11–13]). For a comprehensive review of the related literature on data-driven RANS models, see the review by Duraisamy et al. [14]. Despite the continuous development of RANS closure models to date, none of them ensure mathematical exactness a priori. Therefore, their scope of application is not deterministic, but inevitably open to an empirical study.

Mathematical exactness is a necessary condition for a complete closure of RANS equations, but it is definitely not sufficient. In practice, the mathematically exact relations associated with the Reynolds stress tensor and turbulence quantity transport equations, which have been reported to date, suffer due to the appearance of additional unclosed terms. The needs for modeling were thus inevitably evoked to resolve this under-determinedness. A representative example is the Reynolds stress transport equations, which have unclosed source terms with the exception of the production term. The under-determinedness of these equations seems to have motivated the development of algebraic stress models. Rodi [15] constructed an implicit algebraic stress model by applying an equilibrium hypothesis to the modeled Reynolds stress transport equation of Launder et al. [16]. Since this implicit model requires numerical iterations, it could not be computationally robust [17]. Pope [18] derived an explicit relation for the Reynolds stress tensor by combining the tensorial polynomial expansion thereof with the modeled Reynolds stress transport equation of Rodi [15], but the proposed model is limited to two-dimensional turbulent flow. Gatski and Speziale [19] extended the approach of Pope [18] to three-dimensional turbulent flow by fully considering the ten integrity bases. Further developments were made by introducing near-wall treatments [20] and considering streamline curvature effects [21]. In light of the fundamental reason for the emergence of these algebraic stress models, one may know that the non-appearance of additional unclosed terms is also a necessary condition for the construction of a complete RANS closure.

Most recently, Ryu [22] constructed three identities between Reynolds stresses via spatial mapping and application of the differential Gauss–Bonnet formula [23]. Their methodology is noticeable in two respects: mathematical exactness is ensured by the mathematically proven numerical equality, and the appearance of additional unclosed terms can be prevented by a selective choice of the unit conversion function. However, above all, it is only concerned to the analyticity of a physical scalar field in $\mathbb{R}^3$, which suggests that the methodology can be coherent for both instantaneous and mean flow fields.

In the present paper, the objective is to construct a mathematically exact and well-determined RANS closure. For this task, the incompressible RANS equations are developed into six additional ones by means of the mathematical framework of Ryu [22].

2. Physics-to-Geometry Transformation

We elaborate on the construction process of the mathematical framework of Ryu [22] to help the reader better understand our application of it to RANS equations. Their mathematical framework is constructed in two steps: (i) a physical scalar field of interest is mapped into $\mathbb{R}^3$ and (ii) the differential version of the Gauss–Bonnet formula is applied to the coordinate plane subfields of the mapped field.

In regard to the former, it is the key to convert the unit of the associated physical quantity into that of length. Hereafter, let $G(t, \boldsymbol{x})$ denote a time-dependent, physical scalar field and $D \subseteq \mathbb{R}^3$ be a spatial domain for $G(t, \boldsymbol{x})$, where t is time and $\boldsymbol{x} = (x_1, x_2, x_3)$ are the Cartesian coordinates. The unit of $G(t, \boldsymbol{x})$ may be converted into that of length, as follows:

$$\widetilde{G}(t, \boldsymbol{x}) = G(t, \boldsymbol{x})\sigma(t, \boldsymbol{x}), \tag{2}$$

where σ is the unit-conversion function. Hereafter, we use the overtilde sign $\widetilde{(.)}$ to indicate such a converted field. Then, the respective three subfields of $\widetilde{G}(t, \boldsymbol{x})$ are defined on the three coordinate planes intersecting at each point of D. For example, the converted field $\widetilde{G}$ has three coordinate plane subfields at time t_o and $p_o(x_o, y_o, z_o) \subset D$: $\widetilde{G}(t_o, x, y, z_o)$, $\widetilde{G}(t_o, x, y_o, z)$, $\widetilde{G}(t_o, x_o, y, z)$.

The differential version of the Gauss–Bonnet formula, which has been mathematically proven in Ref. [23], yields three differential equations at p_o for the above-defined three graphs, respectively. The geometric entities of each of those equations are then expanded as introduced in Appendix A. Consequently, this affords three identities in terms only of $\widetilde{G}$ at p_o:

$$\frac{\widetilde{G}_{xx}\widetilde{G}_{yy} - \widetilde{G}_{xy}^2}{\left(1 + \widetilde{G}_x^2 + \widetilde{G}_y^2\right)^{3/2}} + \left\{ \frac{\partial}{\partial x}\left(\frac{-\widetilde{G}_{yy}\widetilde{G}_x}{\left(1 + \widetilde{G}_y^2\right)\sqrt{1 + \widetilde{G}_x^2 + \widetilde{G}_y^2}} \right) - \frac{\partial}{\partial y}\left(\frac{\widetilde{G}_{xx}\widetilde{G}_y}{\left(1 + \widetilde{G}_x^2\right)\sqrt{1 + \widetilde{G}_x^2 + \widetilde{G}_y^2}} \right) \right\} + \frac{\partial^2}{\partial x \partial y}\left\{ \arccos\left(\frac{\widetilde{G}_x\widetilde{G}_y}{\sqrt{1 + \widetilde{G}_x^2}\sqrt{1 + \widetilde{G}_y^2}} \right) \right\} = 0, \tag{3}$$

$$\frac{\widetilde{G}_{zz}\widetilde{G}_{xx} - \widetilde{G}_{zx}^2}{\left(1 + \widetilde{G}_z^2 + \widetilde{G}_x^2\right)^{3/2}} + \left\{ \frac{\partial}{\partial z}\left(\frac{-\widetilde{G}_{xx}\widetilde{G}_z}{\left(1 + \widetilde{G}_x^2\right)\sqrt{1 + \widetilde{G}_z^2 + \widetilde{G}_x^2}} \right) - \frac{\partial}{\partial x}\left(\frac{\widetilde{G}_{zz}\widetilde{G}_x}{\left(1 + \widetilde{G}_z^2\right)\sqrt{1 + \widetilde{G}_z^2 + \widetilde{G}_x^2}} \right) \right\} + \frac{\partial^2}{\partial z \partial x}\left\{ \arccos\left(\frac{\widetilde{G}_z\widetilde{G}_x}{\sqrt{1 + \widetilde{G}_z^2}\sqrt{1 + \widetilde{G}_x^2}} \right) \right\} = 0, \tag{4}$$

$$\frac{\widetilde{G}_{yy}\widetilde{G}_{zz} - \widetilde{G}_{yz}^2}{\left(1 + \widetilde{G}_y^2 + \widetilde{G}_z^2\right)^{3/2}} + \left\{ \frac{\partial}{\partial y}\left(\frac{-\widetilde{G}_{zz}\widetilde{G}_y}{\left(1 + \widetilde{G}_z^2\right)\sqrt{1 + \widetilde{G}_y^2 + \widetilde{G}_z^2}} \right) - \frac{\partial}{\partial z}\left(\frac{\widetilde{G}_{yy}\widetilde{G}_z}{\left(1 + \widetilde{G}_y^2\right)\sqrt{1 + \widetilde{G}_y^2 + \widetilde{G}_z^2}} \right) \right\} + \frac{\partial^2}{\partial y \partial z}\left\{ \arccos\left(\frac{\widetilde{G}_y\widetilde{G}_z}{\sqrt{1 + \widetilde{G}_y^2}\sqrt{1 + \widetilde{G}_z^2}} \right) \right\} = 0, \tag{5}$$

where the subscripts denote the derivatives of $\widetilde{G}$ with respect to x, y, and z, respectively. Note that application of the differential Gauss–Bonnet formula is first considered only at a point of D. For convenience, the left-hand sides of these identities are briefly expressed as the sum of the three budgets:

$$\mathcal{G}\left(x, y; \widetilde{G}(t_o, x, y, z_o)\right) + \Pi\left(x, y; \widetilde{G}(t_o, x, y, z_o)\right) + \Phi\left(x, y; \widetilde{G}(t_o, x, y, z_o)\right) = 0, \tag{6}$$

$$\mathcal{G}\left(z, x; \widetilde{G}(t_o, x, y_o, z)\right) + \Pi\left(z, x; \widetilde{G}(t_o, x, y_o, z)\right) + \Phi\left(z, x; \widetilde{G}(t_o, x, y_o, z)\right) = 0, \tag{7}$$

$$\mathcal{G}\left(y, z; \widetilde{G}(t_o, x_o, y, z)\right) + \Pi\left(y, z; \widetilde{G}(t_o, x_o, y, z)\right) + \Phi\left(y, z; \widetilde{G}(t_o, x_o, y, z)\right) = 0, \tag{8}$$

where $\mathcal{G}$, Π, and Φ are the respective differential operators in order. By adding up the operators of the above equations, respectively, we obtain

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{G}\right)\Big|_{(t_o, p_o)} + \Pi_s\left(\boldsymbol{x}; \widetilde{G}\right)\Big|_{(t_o, p_o)} + \Phi_s\left(\boldsymbol{x}; \widetilde{G}\right)\Big|_{(t_o, p_o)} = 0. \tag{9}$$

Extending the above-described application of the differential Gauss–Bonnet formula to every point of D makes this combined identity applicable as a whole on D:

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{G}(t_o, \mathbf{x})\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{G}(t_o, \mathbf{x})\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{G}(t_o, \mathbf{x})\right) = 0, \ \forall \mathbf{x} \in D. \tag{10}$$

3. Invariance Properties

The above-introduced identity of Equation (10) originates from the differential version of the Gauss–Bonnet formula that concerns only the geometry of an orientable smooth surface in $\mathbb{R}^3$. This implies intriguing invariance properties, which are not dealt with in Ryu [22]. Hereafter, let $\mathcal{R}_s$ denote the sum of $\mathcal{G}_s$, Π_s, and Φ_s.

Lemma 1. *If the coordinate plane subfields of $\widetilde{G}$ are orientable and smooth in $\mathbb{R}^3$ at every instant in time, then the combined identity of Equation (10) is invariant under a shift in time:*

$$\mathcal{R}_s(\boldsymbol{x}; \widetilde{G}(t, \boldsymbol{x})) = \mathcal{R}_s(\boldsymbol{x}; \widetilde{G}(t + \Delta t, \boldsymbol{x})). \tag{11}$$

Lemma 2. *Let $G^*(\boldsymbol{x})$ be a statistic of $G(t, \boldsymbol{x})$ over time and let $\widetilde{G^*}(\boldsymbol{x})$ be the converted field of $G^*(\boldsymbol{x})$ by a time-independent unit conversion function $\sigma(\boldsymbol{x})$. If the coordinate plane subfields of $\widetilde{G^*}$ are orientable and smooth in $\mathbb{R}^3$, then the combined identity of Equation (10) is indifferent to taking a statistic over time:*

$$\mathcal{R}_s(\boldsymbol{x}; \widetilde{G}(t, \boldsymbol{x})) = \mathcal{R}_s(\boldsymbol{x}; \widetilde{G^*}(\boldsymbol{x})). \tag{12}$$

Proof. These two lemmas are proven in Theorem A1. □

Lemma 3. *The combined identity of Equation (10) is invariant under Galilean coordinate transformation.*

Proof. Let $\boldsymbol{x}' = (x', y', z')$ and t' be spatial coordinates and time in the moving frame of reference S' with constant velocity V along the x-direction. Then, the coordinates of $\boldsymbol{x}'$ and time t' are written in terms of the coordinates of $\boldsymbol{x} = (x, y, z)$ and time t in stationary frame of reference S, as follows:

$$x' = x - Vt, \ y' = y, \ z' = z, \ t' = t. \tag{13}$$

These relations give the respective expressions for x, y, and z. In substituting those into Equation (10) and manipulating the derivatives therein, the differential operator $\mathcal{R}_s$ is form-invariant. □

4. Mathematical Formulation

4.1. Generic Formulation

Prior to the construction of a system of equations as a RANS closure, we devise a generic method to derive six additional equations from an established one. To elaborate on this method, first let $\mathbf{A} = \mathbf{B}$ be an equation with rank $r \leq 3$ tensor fields $\mathbf{A}(t, \boldsymbol{x})$ and $\mathbf{B}(t, \boldsymbol{x})$ in $\mathbb{R}^3$.

First, two scalar quantities A and B are defined consistently from $\mathbf{A}$ and $\mathbf{B}$, respectively. For example, in the case of a vector, its magnitude may be chosen as a scalar quantity, and, in the case of a rank-2 tensor, its invariants may afford the scalar quantities. The original equation is then developed into $A = B$.

Second, A and B are converted into a quantity of length by the same unit conversion:

$$\widetilde{A} = A(t, \boldsymbol{x})\sigma_r(t, \boldsymbol{x}), \tag{14}$$

$$\widetilde{B} = B(t, \boldsymbol{x})\sigma_r(t, \boldsymbol{x}). \tag{15}$$

Note that the numerical equality of the developed equation that $A = B$ is retained due to the same unit conversion function:

$$\widetilde{A}(t, \boldsymbol{x}) = \widetilde{B}(t, \boldsymbol{x}). \tag{16}$$

Since there are many possible options about the determination of a unit conversion function, a selective choice is possible for a specific purpose.

The mathematical framework of Equation (10) gives two identities in terms only of $\widetilde{A}$ and $\widetilde{B}$, respectively:

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{A}\right) = 0, \tag{17}$$

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{B}\right) = 0. \tag{18}$$

To derive additional relations between $\widetilde{A}$ and $\widetilde{B}$, it may be a way to selectively substitute $\widetilde{A}$ for $\widetilde{B}$ and vice versa in Equations (17) and (18), respectively. Note that the numerical equality in Equations (17) and (18) is not affected by these substitutions, owing to $\widetilde{A} = \widetilde{B}$. In other words, the numerical equality of $\widetilde{A} = \widetilde{B}$ is a necessary condition for the selectively substituted equations to hold true. The number of all possible cases for such a combinatorial substitution is six. The resulting equations are written as follows:

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{A}\right) = 0, \tag{19}$$

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{A}\right) = 0, \tag{20}$$

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{B}\right) = 0, \tag{21}$$

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{B}\right) = 0, \tag{22}$$

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{A}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{B}\right) = 0, \tag{23}$$

$$\mathcal{G}_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Pi_s\left(\boldsymbol{x}; \widetilde{B}\right) + \Phi_s\left(\boldsymbol{x}; \widetilde{A}\right) = 0. \tag{24}$$

The form of these six equations depends on a chosen unit conversion function. Nonetheless, if it consists only of known variables or simply a constant, the appearance of additional unclosed terms can be avoided. In addition, the mathematical exactness of these equations is ensured by the mathematically proven numerical equality of the differential Gauss–Bonnet formula [23], if the coordinate plane subfields of $\widetilde{A}$ and $\widetilde{B}$ are orientable and smooth in $\mathbb{R}^3$.

4.2. Application to RANS Equations

Taking into consideration that the above-described method gives a total of six additional equations, it is most instructive to apply it to the governing equations for RANS or large-eddy simulation. For the former, the incompressible RANS equations are considered as a target of application in the Cartesian coordinate system:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \tag{25}$$

where U_i is the averaged velocity component along the x_i direction; P is the averaged pressure divided by the fluid density ρ; ν is the kinematic viscosity; and τ_{ij} is the Reynolds stress tensor. The incompressible RANS equations are then developed into a single one by taking divergence on both sides of Equation (25):

$$\frac{\partial^2 \tau_{ij}}{\partial x_i \partial x_j} = -\frac{\partial^2 P}{\partial x_i^2} - \frac{\partial U_j}{\partial x_i}\frac{\partial U_i}{\partial x_j}, \tag{26}$$

The left- and right-hand sides of this reduced equation are briefly written as follows:

$$M(t, \boldsymbol{x}) = F(t, \boldsymbol{x}). \tag{27}$$

Then, M and F are mapped into $\mathbb{R}^3$ by means of the same unit conversion function:

$$\widetilde{M}(t, \boldsymbol{x}) = M(t, \boldsymbol{x})\sigma_r(t, \boldsymbol{x}), \tag{28}$$

$$\widetilde{F}(t, \boldsymbol{x}) = F(t, \boldsymbol{x})\sigma_r(t, \boldsymbol{x}). \tag{29}$$

We choose $\sigma_r = 1$ to avoid appearances of additional unclosed terms and to make the two conversions simplest. Accordingly,

$$\widetilde{M}(t, \boldsymbol{x}) = \widetilde{F}(t, \boldsymbol{x}). \tag{30}$$

Then, this equation is developed into six additional ones through the above-described combinatorial substitutions.

The two constraints for the differential Gauss–Bonnet formula, orientability and smoothness, are not strong to over-constrain the system in question. Since a smooth real scalar function has continuous derivatives of all orders [24] and a surface given by the graph of a differentiable real function is orientable [25], any coordinate subfields of a smooth scalar field in $\mathbb{R}^3$ must be orientable. Accordingly, smoothness is the key necessary condition for the mathematical framework of Equations (3)–(5) to hold true. Taking into consideration that smooth flow fields are common in turbulence, it is difficult to see that the physical quantities described by the proposed equations are significantly distorted by the smoothness constraint.

The numerical equality of the incompressible RANS equations is a necessary condition for the proposed six equations to hold true, as mentioned earlier. Further, the mean continuity equation is applied whilst deriving the mean Poisson equation from the incompressible RANS equations. Therefore, mass and momentum conservation laws are involved in the derivation process of the presented six equations. Moreover, those equations are supposed to be coupled with the mean continuity equation and the incompressible RANS equations in order to obtain ten unknown quantities: one averaged pressure, three averaged velocities, and six Reynolds stress components. Therefore, the proposed six equations are not isolated from mass and momentum conservation laws in solving the ten simultaneous equations.

5. Summary and Concluding Remarks

Six equations have been constructed as a closure for the Reynolds stress tensor by utilizing the mathematical framework of Ryu [22]. The target of application in the present study is distinct from their one; the objects of interest are not Reynolds stresses but the system of RANS equations. The proposed RANS closure is mathematically exact and well-determined, in which it stands out from existing RANS closure models and the Reynolds stress transport equations.

It is extremely challenging to analytically solve the incompressible RANS equations in combination with the presented six equations and the mean continuity equation, owing to their implicitness and double-embedded nonlinearity. By contrast, it seems more feasible to numerically solve these simultaneous equations. Regarding the latter, it would be a first step to set physical boundary conditions for Reynolds stresses in order to close the system of equations. Then, we could aim to find a possibility for obtaining numerically stable and accurate solutions for a benchmark turbulent flow. Despite such a barrier to entry, this is a challenge worth taking on as it could be a pioneering attempt to essentially overcome the inherent limitation of modeling.

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Appendix A. Expansion of Geometric Entity

This Appendix describes the expansions of the geometric entities of the differential Gauss–Bonnet formula for an orientable smooth surface given by parametrization $\mathbf{r} = (u, v, f(u, v))$, $(u, v) \in \mathbb{R}^2$. First, we recall the differential Gauss–Bonnet theorem from Ref. [23].

Theorem A1. *Let S be an orientable smooth surface in $\mathbb{R}^3$, and let $\mathbf{r} : U \to S$ be a parametrization of S in an open set $U \subseteq \mathbb{R}^2$. Then for each $(u, v) \in U$*

$$K|\mathbf{N}| + \left(\frac{\partial F_b}{\partial u} - \frac{\partial F_a}{\partial v}\right) - \frac{\partial^2 \phi}{\partial u \partial v} = 0, \tag{A1}$$

where K is the Gaussian curvature over S, $\mathbf{N}$ is the normal to S, F_a, and F_b are the products of the geodesic curvatures of the coordinate curves $v = const$ and $u = const$ and the speeds of those curves, respectively, and ϕ is the positively oriented angle of intersection from the coordinate curve $v = const$ to $u = const$ on S.

The differential Gauss–Bonnet formula consists of seven geometric entities: K, $|\mathbf{N}|$, $\kappa_{g,u=\text{const}}$, $\kappa_{g,v=\text{const}}$, $|\mathbf{r}_u|$, $|\mathbf{r}_v|$, and ϕ, where κ_g is the geodesic curvature over a coordinate curve on the map of $\mathbf{r}$ and the subscripts u and v denote the first-order derivatives of $\mathbf{r}$ with respect to u and v, respectively. In particular, for a surface given by parametrization $(u, v, f(u, v))$, these are expanded in terms of the derivatives of the two-variable function $f(u, v)$, as follows [25]:

$$K = \frac{f_{uu} f_{vv} - f_{uv}^2}{(1 + f_u^2 + f_v^2)^2}, \tag{A2}$$

$$|\mathbf{N}| = \sqrt{1 + f_u^2 + f_v^2}, \tag{A3}$$

$$|\mathbf{r}_u| = \sqrt{1+f_u^2}, \tag{A4}$$

$$|\mathbf{r}_v| = \sqrt{1+f_v^2}, \tag{A5}$$

$$\kappa_{g,v=\text{const}} = \frac{\langle \mathbf{r}_{uu}, \mathbf{n} \wedge \mathbf{r}_u \rangle}{|\mathbf{r}_u|^3} = \frac{f_{uu} f_v}{(1+f_u^2)^{3/2}\sqrt{1+f_u^2+f_v^2}}, \tag{A6}$$

$$\kappa_{g,u=\text{const}} = \frac{\langle \mathbf{r}_{vv}, \mathbf{n} \wedge \mathbf{r}_v \rangle}{|\mathbf{r}_v|^3} = \frac{-f_{vv} f_u}{(1+f_v^2)^{3/2}\sqrt{1+f_u^2+f_v^2}}, \tag{A7}$$

$$\phi = \arccos\left(\frac{\langle \mathbf{r}_u, \mathbf{r}_v \rangle}{|\mathbf{r}_u||\mathbf{r}_v|}\right) = \arccos\left(\frac{f_u f_v}{\sqrt{1+f_u^2}\sqrt{1+f_v^2}}\right), \tag{A8}$$

where $\mathbf{n}$ is the unit normal to S. The geometric entities of the differential Gauss–Bonnet formula are similarly expandable for the surface given by parametrization $(g(u,v), u, v)$ or $(v, h(u,v), u)$.

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