

Semi-analytical Approach to Three-Dimensional Shape Optimization Problems

Final Performance Report

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Executive Summary

A semi-analytical approach to three-dimensional (3-D) shape optimization problems for a viscous incompressible fluid under the assumption of zero (low) Reynolds number has been developed. It couples the theory of generalized analytic functions with the adjoint equations-based method. A solution to Stokes equations governing the behavior of the fluid has been reduced to integral equations based on the Cauchy integral formula for k -harmonically analytic functions. The fluid velocity and boundary shape are the state and design variables, respectively, and a shape optimization problem is to find shape minimizing the energy dissipation rate. In contrast to the classical optimal control theory, the shape optimization problem has been formulated as an optimal control problem with constraints in the form of integral equations. The optimality conditions (state, adjoint and design equations) for the optimal control problem have been derived. The advantage of the suggested approach is that the state and adjoint variables are single-variable functions, which being represented analytically in the form of series with unknown coefficients, can be accurately determined from the state and adjoint integral equations, for example, by minimizing the total squared error. The optimal shape has been found iteratively by a gradient-based method, in which at each iteration, the state and adjoint variables have been determined for an updated shape and the gradient for the cost functional with respect to the shape has been obtained by the adjoint equations-based method. The suggested semi-analytical approach has been illustrated for the drag minimization problem for motion of a solid body of revolution in the viscous incompressible fluid and has proved to be efficient and accurate.

The project involved two Ph.D. students Anton Molyboha and Bogdan Grechuk from the Department of Mathematical Sciences, Stevens Institute of Technology.

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1. Zabaranin, M. (2008) The framework of k -harmonically analytic functions for three-dimensional Stokes flow problems, Part I, submitted to SIAM Journal on Applied Mathematics
2. Zabaranin, M. (2008) The framework of k -harmonically analytic functions for three-dimensional Stokes flow problems, Part II, submitted to SIAM Journal on Applied Mathematics

1 Introduction

The theory of analytic functions of complex variable is one of the primary methods for analytical treatment of two-dimensional (2-D) problems in various areas of applied mathematics, including the theory of electromagnetism, elasticity and hydrodynamics. Coupled with mathematical programming techniques, it provides an efficient framework for 2-D optimal design problems. This project develops the approach of generalized analytic functions in application to 3-D shape optimization problems, in particular for viscous incompressible fluid. We demonstrated the approach in finding the optimal shape for a solid unit-volume body translating in the fluid with the minimal resistance force (drag).

The behavior of steady flows of a viscous incompressible fluid under the assumption of zero (low) Reynolds number (so-called *Stokes' creeping flows*) is described by the Stokes equations

$$\mu \Delta \mathbf{u} = \text{grad } \wp, \quad \text{div } \mathbf{u} = 0, \quad (1)$$

where $\mathbf{u}$ is the fluid velocity field, $\wp$ is the pressure in the fluid, μ is the shear viscosity, and $\Delta \mathbf{u} \equiv \text{grad}(\text{div } \mathbf{u}) - \text{curl curl } \mathbf{u}$; see [7, 8]. Stokes flows about solid particles have been and continue to be a popular subject of research in fluid mechanics [7], in particular in analytical hydrodynamics. The drag and torque of solid bodies in Stokes flows are used for designing chemical technologies that deal with particle sedimentation; see [7]. Special attention has been paid to the form of a solid body that minimizes the energy dissipation rate in Stokes flows. If the body translates along some axis, e.g., the z -axis, with a constant velocity then the principle of minimizing the energy dissipation rate is equivalent to minimizing the resisting force (drag), experienced by the body. In this regard, the problem of finding the optimal shape for the solid unit-volume body in the Stokes flow is a benchmark problem, which was first addressed by Pironneau [12], who established the optimality condition $\|\frac{\partial \mathbf{u}}{\partial n}\| = \text{const}$ and developed an iterative algorithm for finding the optimal shape. Bourot [3] used Pironneau's algorithm to find the optimal shape and obtained the drag of 0.95425 compared to that of the unit-volume sphere. At each iteration, he represented solution to Stokes equations in the form of the series of spheroidal harmonics¹ and solved the boundary conditions by minimizing the total squared error with respect to unknown coefficients. However, Pironneau's optimality condition is not applicable for incorporating other constraints on the shape and/or motion of the body, e.g., for translation of a solid unit-volume body of revolution in the direction orthogonal to its axis of revolution. Also, implementation of any shape optimization algorithm requires very accurate solution to Stokes equations. To solve this shape optimization problem, Ogawa and Kawahara [11] used the finite element method (FEM). However, their result is visibly different from the one obtained by Bourot. The adjoint equations-based method has proved to be efficient for PDE constrained optimization problems, in particular for control problems in incompressible viscous flows [6]. It makes use of adjoint equations to facilitate finding the gradient for objective function with respect to design variables. For additional details about this shape optimization problem and adjoint equations-based method, see [17, 16, 4, 10, 11, 9, 3, 15, 6, 13, 5, 1, 14].

The goal of this work was to develop efficient algorithms for 3-D shape optimization applicable to different models of the viscous incompressible fluid with a variety of constraints on body's shape (volume, surface, cross-section, etc.) and body's motion. We developed the semi-analytical approach coupling the framework of generalized analytic functions with adjoint equations-based method and demonstrated this approach for the problem of finding optimal shape for the solid unit-volume body translating in the fluid.

In [20], we introduced a special class of generalized analytic functions that arise from the fundamental relationship between a scalar field ϕ and vectorial field $\mathbf{\Lambda}$:

$$\text{grad } \phi = -\text{curl } \mathbf{\Lambda}, \quad \text{div } \mathbf{\Lambda} = 0, \quad (2)$$

¹This solution form is used for representing the velocity field for prolate spheroid.

which maintains that ϕ and $\mathbf{\Lambda}$ are related scalar and vectorial potentials, respectively. This relationship is encountered in various areas of applied mathematics, in particular in hydrodynamics, the theory of elasticity, electromagnetism, etc.; see [20]. With $\text{div } \mathbf{u} = 0$, the first equation in (1) can be rewritten as $\text{grad } \wp = -\mu \text{curl}(\text{curl } \mathbf{u})$, whence it follows that the vorticity $\boldsymbol{\omega} = \text{curl } \mathbf{u}$ and pressure $\wp$ are related by $\text{grad } \wp = -\mu \text{curl } \boldsymbol{\omega}$ with $\text{div } \boldsymbol{\omega} = 0$ and thus, $\mu \boldsymbol{\omega}$ and $\wp$ are related potentials satisfying (2).

In 2-D case in Cartesian coordinates, (2) reduces to the classical Cauchy-Riemann system for ordinary analytic functions, and in the 3-D axially symmetric case in cylindrical coordinates $(r, \varphi, z)^2$, (2) defines so-called r -analytic functions; see [20]. In the 3-D *asymmetric* case, (2) relates the k^{th} harmonics of ϕ and $\mathbf{\Lambda}$, $k \in \mathbb{Z}_0^+$, with respect to φ , and reduces to a series of systems of two linear first-order partial differential equations

$$\left(\frac{\partial}{\partial r} - \frac{k}{r}\right) U^{(k)} = \frac{\partial}{\partial z} V^{(k+1)}, \quad \frac{\partial}{\partial z} U^{(k)} = -\left(\frac{\partial}{\partial r} + \frac{k+1}{r}\right) V^{(k+1)}, \quad (3)$$

which for each $k \in \mathbb{Z}_0^+$ defines a class of k -harmonically analytic functions $G^{(k)}(r, z) = U^{(k)}(r, z) + \mathbf{i} V^{(k+1)}(r, z)$, where $\mathbf{i} = \sqrt{-1}$; see [20].

It follows from (3) that $U^{(k)}$ and $V^{(k+1)}$ are k -harmonic and $(k+1)$ -harmonic functions, respectively, i.e., they satisfy

$$\Delta_k U^{(k)} = 0 \quad \text{and} \quad \Delta_{k+1} V^{(k+1)} = 0, \quad (4)$$

where Δ_k denotes the so-called k -harmonic operator:

$$\Delta_k \equiv \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} - \frac{k^2}{r^2}. \quad (5)$$

In [18, 19], we developed a unifying framework for k -harmonically analytic functions in application to 3-D Stokes flow problems (the papers have been submitted for publication). In particular, we obtained representations for the fluid velocity field in terms of k -harmonically analytic functions in axially symmetric and asymmetric cases and also derived a generalized Cauchy integral formula for k -harmonically analytic functions, which paved the way for reducing 3-D Stokes flow problems to integral equations for k -harmonically analytic functions.³ We formulated the benchmark shape optimization problem as an integral equation constrained optimization problem and solved it using the adjoint equations-based method. As another illustration, we applied the developed approach to shape optimization problem for the solid unit-volume body of revolution translating in the fluid in the direction perpendicular to its axis of revolution. The novelty of the suggested approach is in its accuracy and efficiency.

2 Problem Formulation and Optimality Conditions

Let a solid unit-volume body translate in a viscous incompressible fluid under the assumption of zero (low) Reynolds number with constant velocity v_z along the z -axis. In this case, the fluid velocity field is governed by the Stokes equations (1) and satisfies the no-slip boundary conditions on the surface S of the body and conditions at infinity:

$$\mathbf{u}|_S = v_z \mathbf{k}, \quad \mathbf{u}|_\infty = 0, \quad \wp|_\infty = 0. \quad (6)$$

²In this case, the z -axis is the axis of symmetry, and ϕ and $\mathbf{\Lambda}$ are independent of the angular coordinate φ .

³Another possible approach to solve boundary-value problems for generalized analytic functions is to use formal powers in the sense of Bers [2].

Let $\mathcal{D}_-$ be the domain exterior to the body $\mathcal{D}_+$ ($S = \partial\mathcal{D}_+$). The benchmark shape optimization problem is to minimize the energy dissipation rate in the domain $\mathcal{D}_-$ subject to the boundary conditions (6) (PDE constrained optimization):

$$\begin{aligned} \min_{\partial\mathcal{D}_-} \quad & \iiint_{\mathcal{D}_-} (\text{curl } \mathbf{u})^2 dV \\ \text{s.t.} \quad & \text{Stokes equations (1),} \\ & \text{boundary conditions (6),} \\ & \text{unit volume: } \iiint_{\mathcal{D}_+} dV = 1. \end{aligned} \tag{7}$$

Since the body translates with the constant velocity $v_z \mathbf{k}$, we can represent the energy dissipation rate via the resisting force (drag) $\mathbf{F}$ in the direction of the z -axis

$$\iiint_{\mathcal{D}_-} (\text{curl } \mathbf{u})^2 dV = -v_z \mathbf{k} \cdot \mathbf{F} = -v_z F_z.$$

It follows from the symmetry of F_z , Stokes equations (1) and boundary conditions (6) that the z -axis is body's axis of revolution and thus, the fluid velocity field is axially symmetric, see Figure 1.

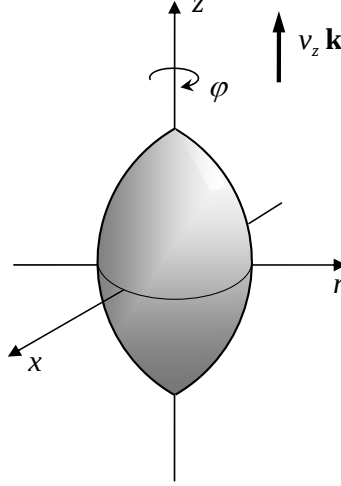


Figure 1: Translation of the solid unit-volume body in the fluid with the velocity v_z along the z -axis.

Let (r, φ, z) be the cylindrical system of coordinates with the basis $(\mathbf{e}_r, \mathbf{e}_\varphi, \mathbf{k})$ and let ℓ_+ be the boundary of the body $\mathcal{D}_+$ in the rz -cross-sectional plane for $r \geq 0$. The components u_r and u_z of the axially symmetric velocity field $\mathbf{u}$ are independent of the angular coordinate φ and $u_\varphi \equiv 0$. Consequently, $\mathbf{u}(r, \varphi, z) = u_r(r, z) \mathbf{e}_r + u_z(r, z) \mathbf{k}$. We also introduce the complex variable $\zeta = r + i z$. In [18], we represented the axially symmetric velocity field $\mathbf{u}$ in terms of two 0-harmonically analytic functions $G_1(\zeta)$ and $G_2(\zeta)$ ⁴:

$$u_z + i u_r = \left(z - \frac{i}{2} r\right) G_1(\zeta) + G_2(\zeta). \tag{8}$$

Thus, the shape optimization problem is to find the boundary ℓ_+ such that minimizes the drag⁵

⁴In our context, the notation $G(\zeta)$ does not assume analyticity of G and simply denotes $G(r, z)$.

⁵In [18], we expressed the drag in terms of the function G_1 .

subject to the boundary conditions formulated in terms of the functions G_1 and G_2 :

$$\begin{aligned} & \min_{\ell_+} \operatorname{Re} \left\{ - \int_{\ell_+} r G_1(\zeta) d\zeta \right\} \\ & \text{s.t. } G_1(\zeta) \text{ and } G_2(\zeta) \text{ are 0-harmonically analytic functions in } \mathcal{D}_-, \\ & \quad \left(z - \frac{i}{2} r \right) G_1(\zeta) + G_2(\zeta) = v_z, \quad \zeta \in \ell_+, \\ & \text{unit volume: } 2\pi \iint_{\ell_+} r dr dz = 1. \end{aligned} \tag{9}$$

There are two issues in dealing with (9): (i) satisfying the condition that $G_1(\zeta)$ and $G_2(\zeta)$ are 0-harmonically analytic functions in $\mathcal{D}_-$, and (ii) finding unknown shape ℓ_+ .

The boundary values of $G_1(\zeta)$ and $G_2(\zeta)$ at ℓ_+ should satisfy the Sokhotsky-Plemelj's formula, which follows from the Cauchy integral formula for k -harmonically analytic functions derived in [18]:

$$\left(2 - \frac{\alpha(\zeta)}{\pi} \right) G_j(\zeta) + \frac{1}{\pi i} \int_{\ell_+} G_j(\tau) \frac{\Omega_+^{(k)}(\zeta, \tau)}{\tau - \zeta} d\tau - \overline{G_j(\tau)} \frac{\Omega_-^{(k)}(\zeta, \tau)}{\bar{\tau} + \zeta} d\bar{\tau} = 0, \quad \zeta \in \ell_+, \quad 1 \leq j \leq 2, \tag{10}$$

where $\Omega_+^{(k)}(\zeta, \tau)$ and $\Omega_-^{(k)}(\zeta, \tau)$ are real-valued functions (see [18]) and $\alpha(\zeta)$ is the angle between the right and left tangent vectors to the curve ℓ_+ at the point ζ . For all points in which ℓ_+ is smooth, $\alpha(\zeta) = \pi$.

In our work [18], we reduced the boundary-value problem $\left(z - \frac{i}{2} r \right) G_1(\zeta) + G_2(\zeta) = v_z$ on ℓ_+ for two 0-harmonically analytic functions $G_1(\zeta)$ and $G_2(\zeta)$ in the domain $\mathcal{D}_-$ to a single integral equation:

$$\mathcal{L}(G_1) = \int_{\ell_+} \left(G_1(\tau) K_1(\zeta, \tau) d\tau - \overline{G_1(\tau)} K_2(\zeta, \tau) d\bar{\tau} \right) = 2v_z, \quad \zeta \in \ell_+, \tag{11}$$

where $\zeta = r + iz$, $\tau = r_1 + iz_1$ and

$$K_1(\zeta, \tau) = \frac{1}{\pi i} C_1(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau), \quad K_2(\zeta, \tau) = \frac{1}{\pi i} C_2(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau) \tag{12}$$

with

$$C_1(\zeta, \tau) = \frac{z_1 - \frac{i}{2} r_1 - (z - \frac{i}{2} r)}{\tau - \zeta}, \quad C_2(\zeta, \tau) = \frac{z_1 + \frac{i}{2} r_1 - (z - \frac{i}{2} r)}{\zeta + \bar{\tau}}.$$

Thus, the problem (9) reduces to

$$\begin{aligned} & \min_{\ell_+} \operatorname{Re} \left\{ - \int_{\ell_+} r G_1(\zeta) d\zeta \right\} \\ & \text{s.t. } \mathcal{L}(G_1) = 2v_z, \quad \zeta \in \ell_+, \\ & \quad 2\pi \iint_{\mathcal{D}_+} r dr dz = 1. \end{aligned} \tag{13}$$

Let the curve ℓ_+ be parameterized by $s \in [0, 1]$, i.e., $\zeta(s) = r(s) + iz(s)$, and let G_1 be determined as a function of s , i.e., $G_1 = G_1(s)$. Then the problem (13) is reformulated as an optimal control problem:

$$\begin{aligned} & \min_{\zeta(s)} \operatorname{Re} \left\{ - \int_0^1 r(s) G_1(s) \dot{\zeta}(s) ds \right\} \\ & \text{s.t. } \mathcal{S}_\zeta(G_1 \dot{\zeta}) = 2v_z, \quad s \in [0, 1], \\ & \quad \pi \int_0^1 r^2(s) \dot{z}(s) ds = 1, \\ & \quad r(0) = 0, \quad r(1) = 0, \end{aligned} \tag{14}$$

where the first constraint is the state equation and the operator $\mathcal{S}_\zeta$ is determined by

$$\mathcal{S}_\zeta(G_1\dot{\zeta}) = \int_0^1 \left(G_1(t) \dot{\zeta}(t) K_1(\zeta(s), \zeta(t)) - \overline{G_1(t)} \overline{\dot{\zeta}(t)} K_2(\zeta(s), \zeta(t)) \right) dt. \quad (15)$$

We also assume that

$$\lim_{s \rightarrow 0} (r(s) G_1(s)) = 0, \quad \lim_{s \rightarrow 1} (r(s) G_1(s)) = 0.$$

Let $\lambda(s)$ be a complex-valued function and let η be a real-valued constant. Then, the Lagrangian for (14) is determined by

$$L(\zeta, \dot{\zeta}; G_1; \bar{\lambda}, \eta) = \operatorname{Re} \left\{ \int_0^1 \left((\mathcal{A}_\zeta(\lambda) - r(s)) G_1(s) \dot{\zeta}(s) - 2v_z \lambda(s) + \eta r^2(s) \dot{z}(s) \right) ds - \frac{\eta}{\pi} \right\}, \quad (16)$$

where

$$\mathcal{A}_\zeta(\lambda) = \int_0^1 \left(\lambda(t) K_1(\zeta(t), \zeta(s)) - \overline{\lambda(t)} \overline{K_2(\zeta(t), \zeta(s))} \right) dt. \quad (17)$$

In this case, the adjoint (or co-state) equation takes the form

$$\mathcal{A}_\zeta(\lambda) = r(s), \quad s \in [0, 1]. \quad (18)$$

With (18), the total variation of the Lagrangian (16) reduces to

$$\begin{aligned} \delta L = \operatorname{Re} \left\{ \int_0^1 \left(G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial r} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial r} + 2\eta r(s) \dot{z}(s) \right) \delta r(s) ds \right. \\ \left. + \int_0^1 \left(G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial z} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial z} - 2\eta r(s) \dot{r}(s) \right) \delta z(s) ds \right\}. \end{aligned} \quad (19)$$

Optimality conditions are summarized below:

$$\text{State eq.:} \quad \underbrace{\int_0^1 \left(G_1(t) \dot{\zeta}(t) K_1(\zeta(s), \zeta(t)) - \overline{G_1(t)} \overline{\dot{\zeta}(t)} K_2(\zeta(s), \zeta(t)) \right) dt}_{\mathcal{S}_\zeta(G_1 \dot{\zeta})} = 2v_z, \quad (20a)$$

$$\text{Adjoint eq.:} \quad \underbrace{\int_0^1 \left(\lambda(t) K_1(\zeta(t), \zeta(s)) - \overline{\lambda(t)} \overline{K_2(\zeta(t), \zeta(s))} \right) dt}_{\mathcal{A}_\zeta(\lambda)} = r(s), \quad (20b)$$

$$\text{Design eq.'s:} \quad \operatorname{Re} \left\{ G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial r} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial r} + 2\eta r(s) \dot{z}(s) \right\} = 0, \quad (20c)$$

$$\operatorname{Re} \left\{ G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial z} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial z} - 2\eta r(s) \dot{r}(s) \right\} = 0, \quad (20d)$$

$$\pi \int_0^1 r^2(s) \dot{z}(s) ds = 1, \quad (20e)$$

$$\text{Boundary cond.'s:} \quad r(0) = 0, \quad r(1) = 0. \quad (20f)$$

Observe that equations (20a)–(20d) are dependent:

$$\begin{aligned} & \dot{r}(s) \left(G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial r} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial r} + 2\eta r(s) \dot{z}(s) \right) \\ & + \dot{z}(s) \left(G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial z} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial z} - 2\eta r(s) \dot{r}(s) \right) \\ & = G_1(s) \dot{\zeta}(s) \frac{d(\mathcal{A}_\zeta(\lambda) - r(s))}{ds} + \lambda(s) \frac{d\mathcal{S}_\zeta(G_1 \dot{\zeta})}{ds} = 0, \end{aligned}$$

whence it follows that

$$\begin{aligned} & G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial z} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial z} - 2\eta r(s) \dot{r}(s) \\ & = -\frac{\dot{r}(s)}{\dot{z}(s)} \left(G_1(s) \dot{\zeta}(s) \frac{\partial(\mathcal{A}_\zeta(\lambda) - r(s))}{\partial r} + \lambda(s) \frac{\partial \mathcal{S}_\zeta(G_1 \dot{\zeta})}{\partial r} + 2\eta r(s) \dot{z}(s) \right). \end{aligned}$$

Solving the system (20a)–(20f) analytically is still an open issue. However, the optimization problem (14) can be efficiently solved by the adjoint equations-based method, which is the subject of the next section.

3 Adjoint Equations-based Method

The problem (14) can be rewritten in the following form

$$\begin{aligned} & \min_{\zeta(s)} \operatorname{Re} \left\{ -\langle G_1 \dot{\zeta}, r \rangle \right\} \\ & \text{s.t. } \mathcal{S}_\zeta(G_1 \dot{\zeta}) = 2v_z, \quad s \in [0, 1], \\ & \quad \zeta(s) \in \mathcal{X}, \end{aligned} \tag{21}$$

where the inner product $\langle \cdot, \cdot \rangle$ is in $\mathcal{L}^2([0, 1])$, i.e., is defined by

$$\langle f, g \rangle = \int_0^1 f(t) \overline{g(t)} dt, \quad \|f\| = \sqrt{\langle f, f \rangle}$$

and

$$\mathcal{X} = \left\{ (r(s), z(s)) \left| \pi \int_0^1 r^2(s) \dot{z}(s) ds = 1, \quad r(0) = 0, \quad r(1) = 0 \right. \right\}. \tag{22}$$

Then the Lagrangian for (21) is given by

$$\begin{aligned} L(\zeta, \dot{\zeta} G_1, \bar{\lambda}) &= \operatorname{Re} \left\{ -\langle G_1 \dot{\zeta}, r \rangle + \langle \mathcal{S}_\zeta(G_1 \dot{\zeta}) - 2v_z, \bar{\lambda} \rangle \right\} \\ &= \operatorname{Re} \left\{ \langle G_1 \dot{\zeta}, \mathcal{S}_\zeta^*(\bar{\lambda}) - r \rangle - \langle 2v_z, \bar{\lambda} \rangle \right\}, \end{aligned} \tag{23}$$

where $\zeta(s) \in \mathcal{X}$ and $\mathcal{S}_\zeta^*$ is the operator adjoint to $\mathcal{S}_\zeta$ and is determined by $\mathcal{S}_\zeta^*(\bar{\lambda}) = \overline{\mathcal{A}_\zeta(\bar{\lambda})}$ (see Appendix A for derivation of the adjoint operator).

The total variation of the Lagrangian takes the form

$$\begin{aligned} \delta L(\zeta, \dot{\zeta} G_1, \bar{\lambda}) &= \operatorname{Re} \{ \langle G_1 \dot{\zeta}, \delta_\zeta(\mathcal{S}_\zeta^*(\bar{\lambda}) - r) \rangle + \langle \delta(G_1 \dot{\zeta}), \mathcal{S}_\zeta^*(\bar{\lambda}) - r \rangle \\ & \quad + \langle \mathcal{S}_\zeta(G_1 \dot{\zeta}) - 2v_z, \delta \bar{\lambda} \rangle \}, \quad \zeta(s) \in \mathcal{X}, \end{aligned}$$

which by the adjoint equations-based method reduces to the variation only with respect to ζ :

$$\begin{aligned} \delta L(\zeta, \dot{\zeta} G_1, \bar{\lambda}) &= \delta_\zeta L = \operatorname{Re}\{\langle \delta_\zeta \mathcal{S}_\zeta(G_1 \dot{\zeta}), \bar{\lambda} \rangle - \langle G_1 \dot{\zeta}, \delta r \rangle\} \\ \text{s.t. state eq.:} \quad &\mathcal{S}_\zeta(G_1 \dot{\zeta}) = 2v_z, \\ \text{adjoint eq.:} \quad &\mathcal{S}_\zeta^*(\bar{\lambda}) = r, \\ &\zeta(s) \in \mathcal{X}, \end{aligned}$$

where

$$\delta_\zeta \mathcal{S}_\zeta(f) = \int_0^1 \left(f(t) \delta K_1(\zeta(s), \zeta(t)) - \overline{f(t)} \delta K_2(\zeta(s), \zeta(t)) \right) dt$$

and

$$\delta K_j(\zeta, \tau) = \frac{\partial K_j(\zeta, \tau)}{\partial r} \delta r + \frac{\partial K_j(\zeta, \tau)}{\partial r_1} \delta r_1 + \frac{\partial K_j(\zeta, \tau)}{\partial z} \delta z + \frac{\partial K_j(\zeta, \tau)}{\partial z_1} \delta z_1, \quad j = 1, 2.$$

The corresponding derivatives of K_1 and K_2 are presented in Appendix B.

The variation of the Lagrangian is used to find the direction $\delta\zeta$ in which the drag value has the steepest descent. Let

$$F(\delta\zeta) = \operatorname{Re}\{\langle \delta_\zeta \mathcal{S}_\zeta(G_1 \dot{\zeta}), \bar{\lambda} \rangle - \langle G_1 \dot{\zeta}, \delta r \rangle\},$$

which is a linear operator with respect to $\delta\zeta$, and let

$$\zeta(s) = \gamma \hat{\zeta}(s) = \gamma \sum_{j=1}^n a_j \hat{\zeta}_j(s) \in \mathcal{X}, \quad (24)$$

where $\hat{\zeta}_j(s)$ are basis functions and $\gamma = \gamma(a_1, \dots, a_n)$ is the multiplier chosen to satisfy the unit-volume constraint. Then we can write

$$\delta\zeta = \sum_{j=1}^n (a_j \delta\gamma + \gamma \delta a_j) \hat{\zeta}_j(s) = \sum_{j=1}^n b_j \hat{\zeta}_j(s),$$

where $b_j = a_j \sum_{i=1}^n \frac{\partial \gamma}{\partial a_i} \delta a_i + \gamma \delta a_j$, or in vectorial notation, if $\mathbf{a} = (a_1, \dots, a_n)^\top$, $\mathbf{d} = (\delta a_1, \dots, \delta a_n)^\top$ and $\mathbf{b} = (b_1, \dots, b_n)^\top$, then $\mathbf{b} = (\nabla \gamma \cdot \mathbf{d}) \mathbf{a} + \gamma \mathbf{d}$. In terms of (24), the unit-volume constraint takes the form $\pi \gamma^3 \int_0^1 \hat{r}^2(s) \hat{z}(s) ds = 1$ and thus, the gradient of γ with respect to $\mathbf{a}$ is determined by

$$\frac{\partial \gamma}{\partial a_j} = - \frac{\int_0^1 \left(2 \hat{r}_j(s) \hat{r}(s) \hat{z}(s) + \hat{r}^2(s) \hat{z}_j(s) \right) ds}{3\pi^{1/3} \left(\int_0^1 \hat{r}^2(s) \hat{z}(s) ds \right)^{4/3}}. \quad (25)$$

From (25), we have $(\nabla \gamma \cdot \mathbf{a}) = -\gamma$, whence $(\nabla \gamma \cdot \mathbf{b}) = (\nabla \gamma \cdot \mathbf{d})(\nabla \gamma \cdot \mathbf{a}) + \gamma(\nabla \gamma \cdot \mathbf{d}) = 0$.

To find the direction $\mathbf{d}^*$ of the steepest descent, we formulate the following problem

$$\min_{\|\delta\zeta\|=1} F(\delta\zeta) = \min_{\mathbf{b}} (\mathbf{f} \cdot \mathbf{b}) \quad \text{subject to} \quad \mathbf{b}^\top H \mathbf{b} = 1, \quad (\nabla \gamma \cdot \mathbf{b}) = 0, \quad (26)$$

where the vector $\mathbf{f}$ has components $f_j = F(\hat{\zeta}_j)$, H is the symmetric matrix with elements $H_{ij} = \langle \hat{\zeta}_i, \hat{\zeta}_j \rangle$ and $G_1(s)$ and $\lambda(s)$ are found from the state and adjoint equations, respectively (this will be discussed in the end of the section). Solving (26), we obtain

$$\mathbf{b}^* = \left(\mathbf{f}^\top H^{-1} \mathbf{f} - \frac{(\nabla \gamma^\top H^{-1} \mathbf{f})^2}{\nabla \gamma^\top H^{-1} \nabla \gamma} \right)^{-1} \left(\frac{\nabla \gamma^\top H^{-1} \mathbf{f}}{\nabla \gamma^\top H^{-1} \nabla \gamma} H^{-1} \nabla \gamma - H^{-1} \mathbf{f} \right),$$

and consequently, we can express $\mathbf{d}$ via $\mathbf{b}$ as

$$\mathbf{d}^* = \frac{1}{\gamma} (\mathbf{b}^* - (\nabla \gamma \cdot \mathbf{d}^*) \mathbf{a}). \quad (27)$$

Since the scalar product of (27) with $\nabla\gamma$ reduces to identity, $\mathbf{d}^*$ can be chosen so that $(\nabla\gamma \cdot \mathbf{d}^*) = 0$.

Then the new vector $\mathbf{a}_{\text{new}}$ is determined by

$$\mathbf{a}_{\text{new}} = \mathbf{a} + h \mathbf{d}^*,$$

where the step size h is found by the golden section technique.

Finally, representing the functions $G_1(s)$ and $\lambda(s)$ on $[0, 1]$ in the form

$$\begin{aligned} G_1(s) &= \sum_{k=1}^m (p_{1k} \widehat{g}_{1k}(s) + i p_{2k} \widehat{g}_{2k}(s)), \\ \lambda(s) &= \sum_{k=1}^m (q_{1k} \widehat{\lambda}_{1k}(s) + i q_{2k} \widehat{\lambda}_{2k}(s)), \end{aligned} \quad (28)$$

where $\widehat{g}_{1k}(s)$, $\widehat{g}_{2k}(s)$, $\widehat{\lambda}_{1k}(s)$ and $\widehat{\lambda}_{2k}(s)$ are basis functions, satisfying the boundary conditions $r(0) = 0$ and $r(1) = 0$ and the symmetry conditions $G_1(1-s) = -\overline{G_1(s)}$ and $\lambda(1-s) = -\overline{\lambda(s)}$, we find unknown coefficients p_{1k} , p_{2k} , q_{1k} and q_{2k} by minimizing the total squared error

$$\min_{p_{1k}, p_{2k}} \|\mathcal{S}_\zeta(G_1\dot{\zeta}) - 2v_z\|^2, \quad \min_{q_{1k}, q_{2k}} \|\mathcal{S}_\zeta^*(\bar{\lambda}) - r\|^2, \quad (29)$$

where $\|\cdot\|$ is the norm in $\mathcal{L}^2([0, 1])$.

Let the coefficients $p_{11}, \dots, p_{1m}, p_{21}, \dots, p_{2m}$ form single vector $\mathbf{p}$ and let a matrix J consist of four blocks, each of which having the components

$$\begin{aligned} J_{jk}^I &= \text{Re}\{\langle \mathcal{S}_\zeta(\dot{\zeta} \widehat{g}_{1j}(s)), \mathcal{S}_\zeta(\dot{\zeta} \widehat{g}_{1k}(s)) \rangle\}, & J_{jk}^{II} &= \text{Re}\{\langle \mathcal{S}_\zeta(\dot{\zeta} \widehat{g}_{1j}(s)), \mathcal{S}_\zeta(i \dot{\zeta} \widehat{g}_{2k}(s)) \rangle\}, \\ J_{jk}^{III} &= J_{kj}^{II}, & J_{jk}^{IV} &= \text{Re}\{\langle \mathcal{S}_\zeta(i \dot{\zeta} \widehat{g}_{2j}(s)), \mathcal{S}_\zeta(i \dot{\zeta} \widehat{g}_{2k}(s)) \rangle\}. \end{aligned}$$

Also let components

$$w_k = 2v_z \text{Re}\{\langle 1, \mathcal{S}_\zeta(\dot{\zeta} \widehat{g}_{1k}(s)) \rangle\}, \quad w_{m+k} = 2v_z \text{Re}\{\langle 1, \mathcal{S}_\zeta(i \dot{\zeta} \widehat{g}_{2k}(s)) \rangle\}, \quad 1 \leq k \leq m,$$

form vector $\mathbf{w}$, then the first problem in (29) reduces to a simple quadratic optimization problem

$$\min_{\mathbf{p}} \mathbf{p}^\top J \mathbf{p} - 2\mathbf{w}^\top \mathbf{p}, \quad (30)$$

whose solution is given by $\mathbf{p} = J^{-1} \mathbf{w}$. The second minimization problem in (29) is solved similarly.

We summarize the adjoint equations-based method for finding the optimal shape.

Algorithm 1

1. Parametrize $\zeta(s) = \gamma(a_1, \dots, a_n) \sum_{j=1}^n a_j \widehat{\zeta}_j(s) \in \mathcal{X}$ and set initial $\mathbf{a} = (a_1, \dots, a_n)$,
2. Solve the state and adjoint equations for a given shape ζ by minimizing the total squared error (problem (29)),
3. Calculate the optimal direction $\mathbf{d}^*$ by (27),
4. Find the optimal step h in the direction $\mathbf{d}^*$ and update $\mathbf{a}$,
5. If $\|h \mathbf{d}^*\| < \epsilon$ then Stop, otherwise Go To Step 2.

The next section implements the algorithm and presents computational results.

4 Computational Results

Let body's shape be represented in the form

$$\zeta(s) = i\gamma \sum_{k=1}^n a_k e^{-\pi i s} T_{2k-2}(2s-1), \quad s \in [0, 1], \quad (31)$$

where $T_k(t)$ are Chebyshev's polynomials of the first kind and the multiplier $\gamma = \gamma(a_1, \dots, a_n)$ is found from the constraint $\pi\gamma^3 \int_0^1 \hat{r}^2(s) \hat{z}(s) ds = 1$ (unit volume). Obviously, $r(0) = 0$ and $r(1) = 0$.

Solutions to the state and adjoint equations are found from (28) with

$$\begin{aligned} \hat{g}_{1k}(s) &= T_{2k-1}(2s-1), & \hat{g}_{2k}(s) &= T_{2k-2}(2s-1), & 1 \leq k \leq m, \\ \hat{\lambda}_{1k}(s) &= T_{2k-1}(2s-1), & \hat{\lambda}_{2k}(s) &= T_{2k-2}(2s-1), & 1 \leq k \leq m. \end{aligned} \quad (32)$$

We solved the shape optimization problem for $m = 12$ starting from the unit-volume sphere. For the first iteration, we used $n = 2$ in the basis $\{\hat{\zeta}_k(t)\}_{k=1}^n$ and then after each 3 iterations, we increased n by 1. This adaptive basis procedure proved to be very efficient. We obtained the drag value of 0.95426 after 8 iterations (this value is normalized to the drag of the unit-volume sphere).⁶ Figure 2 plots the objective function against iteration number. For example, after 13 iterations ($n = 6$), we obtained the drag of 0.954258 and the following shape:

$$\begin{aligned} \gamma &= 0.5988558320119997, \\ a_1 &= 1.294644111408456, \quad a_2 = 0.4790126176431742, \quad a_3 = 0.02076294285722642, \\ a_4 &= -0.008671329483245576, \quad a_5 = -0.002115187983386224, \quad a_5 = -0.00024273396227855588. \end{aligned}$$

Figure 3 shows the optimal shape for the solid unit-volume body translating in the fluid with constant velocity and minimal drag. The shape is (almost) identical to the one obtained by Bourot [3] and is a significant improvement compared to the result of Ogawa and Kawahara [11].

As expected, the performance of the algorithm, which is gradient-based, depends on the initial choice of the shape and on the method for finding optimal step size for a given direction. As an improvement for the algorithm, we can employ a conjugate gradient method, which uses the information about several consecutive gradients.

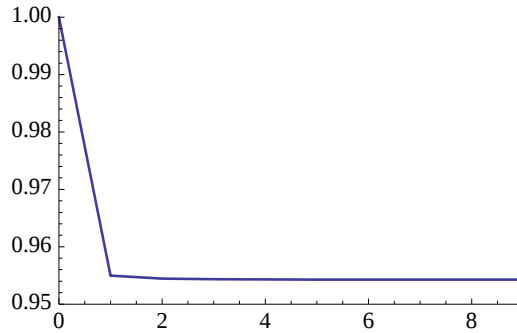


Figure 2: Value of the objective function, normalized to the drag of the unit-volume sphere, for each iteration. The drag value of 0.95426 was obtained after 8 iterations ($m = 12$ and $n = 5$) by adaptive basis procedure.

⁶Bourot's value is 0.95425; see [3].

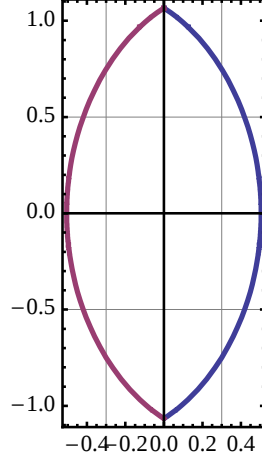


Figure 3: Optimal shape for the solid unit-volume body translating in the fluid with constant velocity and the drag of 0.95426 ($m = 12$, $n = 5$, 8 iterations).

5 Optimal Shape for Transversal Translation

In this section, we solve the problem of finding optimal shape for a solid unit-volume body of revolution translating in a viscous incompressible fluid in the direction transversal to the axis of revolution. To the best of our knowledge, this problem has not been addressed. As in the previous case, we minimize the energy dissipation rate subject to the condition that the fluid velocity field is governed by the Stokes equations (1). Here, we assume that the z -axis is body's axis of revolution and that the body translates along the y -axis with the constant velocity $v_y \mathbf{j}$; see Figure 4. In this case, the boundary conditions for the velocity field are given by

$$\mathbf{u}|_S = v_y \mathbf{j}, \quad \mathbf{u}|_\infty = 0, \quad \varphi|_\infty = 0. \quad (33)$$

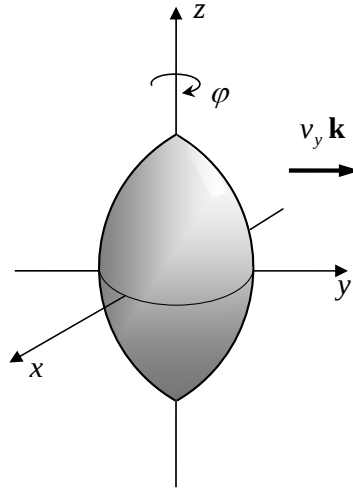


Figure 4: Transversal translation of the solid unit-volume body of revolution in the fluid.

The shape optimization problem is formulated similarly to the problem (7) (PDE constrained

optimization):

$$\begin{aligned}
& \min_{\partial \mathcal{D}_-} \iiint_{\mathcal{D}_-} (\operatorname{curl} \mathbf{u})^2 dV \\
& \text{s.t.} \quad \text{Stokes equations (1),} \\
& \quad \text{boundary conditions (33),} \\
& \quad \text{unit volume: } \iiint_{\mathcal{D}_+} dV = 1, \\
& \quad z\text{-axis is body's axis of revolution,}
\end{aligned}$$

where $\mathcal{D}_+$ and $\mathcal{D}_-$ denote interior and exterior domains for the body, respectively.

As in the previous case, since the body translates with the constant velocity $v_y \mathbf{j}$, we can represent the energy dissipation rate via the resisting force (drag) $\mathbf{F}$ in the direction of the y -axis

$$\iiint_{\mathcal{D}_-} (\operatorname{curl} \mathbf{u})^2 dV = -v_y \mathbf{j} \cdot \mathbf{F} = -v_y F_y.$$

In our work [19], we reduced the Stokes equations (1) for the boundary conditions (33) to two integral equations using Sokhotsky-Plemelj's formula (10) for k -harmonically analytic functions. Consequently, the shape optimization problem reduces to minimizing the drag subject to two integral equation constraints:

$$\begin{aligned}
& \min_{\zeta(s)} \operatorname{Re} \left\{ -\langle G_1^{(0)} \dot{\zeta}, r \rangle \right\} \\
& \text{s.t.} \quad G_1^{(0)}(s) = H_1(s) + \mathbf{i} H_2(s) \\
& \quad G_2(s) = \tfrac{1}{2} r H_2(s) + \mathbf{i} H_3(s), \\
& \quad \mathcal{T}_\zeta(G_1^{(0)} \dot{\zeta}) + \mathcal{P}_\zeta(G_2 \dot{\zeta}) = -4v_y, \quad s \in [0, 1], \\
& \quad \operatorname{Re}\{\beta(s) G_2(s) + \mathcal{R}_\zeta(G_2 \dot{\zeta})\} = 0, \quad s \in [0, 1], \\
& \quad \zeta(s) \in \mathcal{X},
\end{aligned} \tag{34}$$

where $\zeta = r + \mathbf{i} z$ and $\tau = r_1 + \mathbf{i} z_1$ are complex variables in the rz -cross-sectional plane in the cylindrical coordinates (r, φ, z) , in which the z -axis coincides with the z -axis in the Cartesian coordinates (x, y, z) ; $H_1(s)$, $H_2(s)$ and $H_3(s)$ are unknown real-valued functions⁷ parametrized by s on $[0, 1]$; $\beta(s) = 2 - \frac{\alpha(\zeta(s))}{\pi}$ with $\alpha(\zeta)$ same as in (10); and

$$\begin{aligned}
\mathcal{T}_\zeta(G_1^{(0)} \dot{\zeta}) &= \int_0^1 \left(G_1^{(0)}(t) \dot{\zeta}(t) M_1(\zeta(s), \zeta(t)) - \overline{G_1^{(0)}(t) \dot{\zeta}(t)} M_2(\zeta(s), \zeta(t)) \right) dt, \\
\mathcal{P}_\zeta(G_2 \dot{\zeta}) &= \int_0^1 \left(G_2(t) \dot{\zeta}(t) M_3(\zeta(s), \zeta(t)) - \overline{G_2(t) \dot{\zeta}(t)} M_4(\zeta(s), \zeta(t)) \right) dt, \\
M_1(\zeta, \tau) &= \frac{1}{\pi \mathbf{i}} C_{11}(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau), \quad M_2(\zeta, \tau) = \frac{1}{\pi \mathbf{i}} C_{21}(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau), \\
C_{11}(\zeta, \tau) &= \frac{z - z_1 - 2\mathbf{i}(r - r_1)}{\tau - \zeta}, \quad C_{21}(\zeta, \tau) = \frac{z - z_1 - 2\mathbf{i}(r + r_1)}{\bar{\tau} + \zeta}, \\
M_3(\zeta, \tau) &= \frac{1}{\pi \mathbf{i}} \frac{\Omega_+^{(0)}(\zeta, \tau) - \Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta}, \quad M_4(\zeta, \tau) = \frac{1}{\pi \mathbf{i}} \frac{\Omega_-^{(0)}(\zeta, \tau) + \Omega_-^{(1)}(\zeta, \tau)}{\bar{\tau} + \zeta},
\end{aligned}$$

⁷In [19], the functions $H_1(s)$, $H_2(s)$ and $H_3(s)$ correspond to $U_1^{(0)}(s)$, $V_1^{(1)}(s)$ and $U_3^{(0)}(s)$, respectively.

$$\mathcal{R}_\zeta(G_2\dot{\zeta}) = \frac{1}{\pi i} \int_0^1 \left(G_2(t) \dot{\zeta}(t) \frac{\Omega_+^{(1)}(\zeta(s), \zeta(t))}{\zeta(t) - \zeta(s)} + \overline{G_2(t) \dot{\zeta}(t)} \frac{\Omega_-^{(1)}(\zeta(s), \zeta(t))}{\overline{\zeta(t)} + \zeta(s)} \right) dt,$$

and the set $\mathcal{X}$ is defined by (22).

We solved the problem (34) using the adjoint equations-based method discussed in Section 3.

Let $\lambda_1(s) \in \mathbb{C}$ and $\lambda_2(s) \in \mathbb{R}$, then the Lagrangian for (34) takes the form

$$\begin{aligned} L(\zeta, H_1, H_2, H_3, \bar{\lambda}_1, \lambda_2) &= \text{Re} \left\{ -\langle G_1^{(0)} \dot{\zeta}, r \rangle + \langle \mathcal{T}_\zeta(G_1^{(0)} \dot{\zeta}) + \mathcal{P}_\zeta(G_2 \dot{\zeta}) - 4v_y, \bar{\lambda}_1 \rangle + \langle \beta G_2 + \mathcal{R}_\zeta(G_2 \dot{\zeta}), \lambda_2 \rangle \right\} \\ &= \text{Re} \left\{ \langle H_1, \bar{\zeta}(\mathcal{T}_\zeta^*(\bar{\lambda}_1) - r) \rangle + \langle H_3, -i\bar{\zeta}(\mathcal{P}_\zeta^*(\bar{\lambda}_1) + \mathcal{R}_\zeta^*(\lambda_2)) - i\beta \lambda_2 \rangle - 4v_y \langle \lambda_1, 1 \rangle \right. \\ &\quad \left. + \langle H_2, -i\bar{\zeta}(\mathcal{T}_\zeta^*(\bar{\lambda}_1) - r) + \frac{r}{2} \bar{\zeta}(\mathcal{P}_\zeta^*(\bar{\lambda}_1) + \mathcal{R}_\zeta^*(\lambda_2)) + \frac{r}{2} \beta \lambda_2 \rangle \right\}, \end{aligned}$$

whence it follows that the adjoint equations are

$$\begin{aligned} \text{Re} \left\{ \bar{\zeta}(\mathcal{T}_\zeta^*(\bar{\lambda}_1) - r) \right\} &= 0, \\ \text{Re} \left\{ -i\bar{\zeta}(\mathcal{T}_\zeta^*(\bar{\lambda}_1) - r) + \frac{r}{2} \bar{\zeta}(\mathcal{P}_\zeta^*(\bar{\lambda}_1) + \mathcal{R}_\zeta^*(\lambda_2)) + \frac{r}{2} \beta \lambda_2 \right\} &= 0, \\ \text{Re} \left\{ -i\bar{\zeta}(\mathcal{P}_\zeta^*(\bar{\lambda}_1) + \mathcal{R}_\zeta^*(\lambda_2)) - i\beta \lambda_2 \right\} &= 0, \end{aligned}$$

or equivalently,

$$\text{Re} \left\{ \dot{\zeta}(\overline{\mathcal{T}_\zeta^*(\bar{\lambda}_1) - r}) \right\} = 0, \quad \dot{\zeta} \left(\overline{\mathcal{T}_\zeta^*(\bar{\lambda}_1) - r} - \frac{i}{2} r(\overline{\mathcal{P}_\zeta^*(\bar{\lambda}_1) + \mathcal{R}_\zeta^*(\lambda_2)}) \right) - \frac{i}{2} r \beta \lambda_2 = 0, \quad (35)$$

where $\mathcal{T}_\zeta^*$, $\mathcal{P}_\zeta^*$ and $\mathcal{R}_\zeta^*$ are adjoint operators determined by (see Appendix A)

$$\begin{aligned} \overline{\mathcal{T}_\zeta^*(\bar{\lambda}_1)} &= \int_0^1 \left(\lambda_1(t) M_1(\zeta(t), \zeta(s)) - \overline{\lambda_1(t)} \overline{M_2(\zeta(s), \zeta(t))} \right) dt, \\ \overline{\mathcal{P}_\zeta^*(\bar{\lambda}_1)} &= \int_0^1 \left(\lambda_1(t) M_3(\zeta(s), \zeta(t)) - \overline{\lambda_1(t)} \overline{M_4(\zeta(s), \zeta(t))} \right) dt, \\ \overline{\mathcal{R}_\zeta^*(\lambda_2)} &= -\frac{1}{\pi i} \int_0^1 \left(\lambda_2(t) \frac{\Omega_+^{(1)}(\zeta(t), \zeta(s))}{\zeta(t) - \zeta(s)} + \overline{\lambda_2(t)} \frac{\Omega_-^{(1)}(\zeta(t), \zeta(s))}{\overline{\zeta(t)} + \zeta(s)} \right) dt. \end{aligned}$$

Using the adjoint equations-based method, we can write the total variation of the Lagrangian only with respect to ζ and $\dot{\zeta}$:

$$\begin{aligned} \delta_{\zeta, \dot{\zeta}} L &= \text{Re} \left\{ -\langle G_1^{(0)} \delta \dot{\zeta}, r \rangle - \langle G_1^{(0)} \dot{\zeta}, \delta r \rangle + \langle \mathcal{T}_\zeta(G_1^{(0)} \delta \dot{\zeta}) + \mathcal{P}_\zeta(G_2 \delta \dot{\zeta}), \bar{\lambda}_1 \rangle + \langle \mathcal{R}_\zeta(G_2 \delta \dot{\zeta}), \lambda_2 \rangle \right. \\ &\quad \left. + \langle \delta_\zeta \mathcal{T}_\zeta(G_1^{(0)} \dot{\zeta}) + \delta_\zeta \mathcal{P}_\zeta(G_2 \dot{\zeta}), \bar{\lambda}_1 \rangle + \langle \frac{\beta}{2} H_2 \delta r + \delta_\zeta \mathcal{R}_\zeta(G_2 \dot{\zeta}), \lambda_2 \rangle \right\} \end{aligned}$$

subject to the constraints in (34) and adjoint equations (35). Here we have

$$\begin{aligned} \delta_\zeta \mathcal{T}_\zeta(G_1^{(0)} \dot{\zeta}) &= \int_0^1 \left(G_1^{(0)}(t) \dot{\zeta}(t) \delta M_1(\zeta(s), \zeta(t)) - \overline{G_1^{(0)}(t) \dot{\zeta}(t)} \delta M_2(\zeta(s), \zeta(t)) \right) dt, \\ \delta_\zeta \mathcal{P}_\zeta(G_2 \dot{\zeta}) &= \int_0^1 \left(G_2(t) \dot{\zeta}(t) \delta M_3(\zeta(s), \zeta(t)) - \overline{G_2(t) \dot{\zeta}(t)} \delta M_4(\zeta(s), \zeta(t)) \right) dt + \mathcal{P}_\zeta(\frac{1}{2} H_2 \dot{\zeta} \delta r), \end{aligned}$$

$$\begin{aligned}\delta_\zeta \mathcal{R}_\zeta(G_2 \dot{\zeta}) &= \frac{1}{\pi i} \int_0^1 \left(G_2(t) \dot{\zeta}(t) \delta \left(\frac{\Omega_+^{(1)}(\zeta(s), \zeta(t))}{\zeta(t) - \zeta(s)} \right) + \overline{G_2(t) \dot{\zeta}(t)} \delta \left(\frac{\Omega_-^{(1)}(\zeta(s), \zeta(t))}{\overline{\zeta(t)} + \zeta(s)} \right) \right) dt \\ &\quad + \mathcal{R}_\zeta \left(\frac{1}{2} H_2 \dot{\zeta} \delta r \right),\end{aligned}$$

where

$$\delta M_j(\zeta, \tau) = \frac{\partial M_j(\zeta, \tau)}{\partial r} \delta r + \frac{\partial M_j(\zeta, \tau)}{\partial r_1} \delta r_1 + \frac{\partial M_j(\zeta, \tau)}{\partial z} \delta z + \frac{\partial M_j(\zeta, \tau)}{\partial z_1} \delta z_1, \quad j = 1, 2.$$

The corresponding derivatives of M_j are presented in Appendix C.

We represented $\zeta(s)$ in the form similar to (31)

$$\begin{aligned}\zeta(s) &= i\gamma \sum_{k=1}^n a_k e^{-\pi i s} T_{2k-2}(2s), \quad s \in [0, \tfrac{1}{2}], \\ \zeta(s) &= \overline{\zeta(1-s)}, \quad s \in [\tfrac{1}{2}, 1],\end{aligned}\tag{36}$$

which in contrast to (31) allows for non-smoothness at $s = \frac{1}{2}$, and calculated the gradient as in Section 3. Since the state and adjoint variables satisfy the following symmetry conditions

$$\begin{aligned}H_1(1-s) &= -H_1(s), \quad H_2(1-s) = H_2(s), \quad H_3(1-s) = -H_3(s), \\ \lambda_1(1-s) &= \overline{\lambda_1(s)}, \quad \lambda_2(1-s) = \lambda_2(s),\end{aligned}$$

we represented them on $[0, \frac{1}{2}]$ in the form of series with Chebyshev's polynomials of the first kind (similar to (28) with (32)) and found unknown coefficients by minimizing the total squared error (see the problem (29)).

In our preliminary numerical experiments, we obtained the optimal drag of 0.9877, normalized to the drag of the unit-volume sphere, for $m = 9$ and $n = 4$ and expect that this result can be improved. The shape that corresponds to this value is determined by

$$\begin{aligned}\gamma &= 0.6192260666309106, \\ a_1 &= 0.9994918803923275, \quad a_2 = 0.18824077143133067, \\ a_3 &= -0.01408994670305956, \quad a_4 = 0.0066332158943282656,\end{aligned}$$

and is shown in Figure 5.

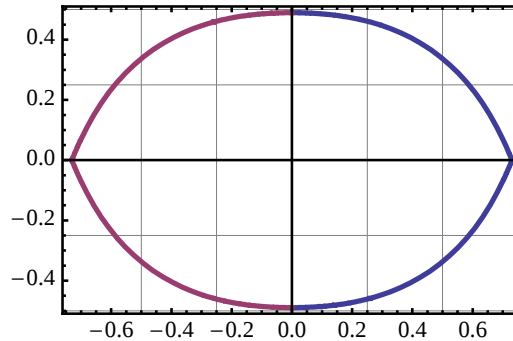


Figure 5: Preliminary results: optimal shape for the solid unit-volume body of revolution translating in the fluid with constant velocity in the horizontal direction (vertical axis is the axis of revolution, and $m = 9$ and $n = 4$).

6 Conclusions

We have suggested the semi-analytical approach to three-dimensional (3-D) shape optimization problems. The approach couples the framework of the generalized analytic functions with adjoint equations-based method and is summarized below.

- (i) Identify the class of generalized analytic functions related to the governing equations (e.g., Stokes equations, Oseen equations, Maxwell's equations, etc.),
- (ii) Represent solution to the governing equations in terms of the generalized analytic functions,
- (iii) Use the Cauchy integral formula for the generalized analytic functions to reduce boundary-value problems for governing equations to corresponding integral equations (state equations),
- (iv) Formulate shape optimization problem with integral equation constraints and apply adjoint equations-based method for obtaining the gradient of the Lagrangian,
- (v) Solve the state and adjoint equations by minimizing the total squared error.

We have illustrated this approach in solving drag minimization problem for a solid unit-volume body translating in a viscous incompressible fluid with constant velocity under the assumption of zero (low) Reynolds number. We have also solved this problem under the constraint that the body has the axis of revolution and translates in the direction perpendicular to the axis. The novelty and advantage of the approach is in its efficiency and accuracy, which can be attributed to

- Solution on the boundary versus solution in the domain (PDE constrained optimization),
- Analytical representations for the state and adjoint functions and for body's shape,
- Analytical form of the gradient.

Among open issues are those inherited from the gradient-based method, namely

- Finding global optimum vs. local optimum, and
- Finding initial shape efficiently.

Addressing these issues as well as applying the developed approach to other physical models, e.g., to Maxwell's equations governing the behavior of electromagnetic waves, are the subject for the future research.

A Derivation of the Adjoint Operator

Let $\mathcal{S}_\zeta(f) = \int_0^1 \left(f(t) K_1(\zeta(s), \zeta(t)) - \overline{f(t)} K_2(\zeta(s), \zeta(t)) \right) dt$ then

$$\begin{aligned}
 \operatorname{Re}\{\langle \mathcal{S}_\zeta(f), \bar{\lambda} \rangle\} &= \operatorname{Re} \left\{ \int_0^1 \lambda(s) \int_0^1 \left(f(t) K_1(\zeta(s), \zeta(t)) - \overline{f(t)} K_2(\zeta(s), \zeta(t)) \right) dt ds \right\} \\
 &= \operatorname{Re} \left\{ \int_0^1 f(s) \int_0^1 \lambda(t) K_1(\zeta(t), \zeta(s)) dt ds - \int_0^1 \overline{f(s)} \int_0^1 \lambda(t) K_2(\zeta(t), \zeta(s)) dt ds \right\} \\
 &= \operatorname{Re} \left\{ \int_0^1 f(s) \int_0^1 \left(\lambda(t) K_1(\zeta(t), \zeta(s)) - \overline{\lambda(t)} \overline{K_2(\zeta(t), \zeta(s))} \right) dt ds \right\} \\
 &= \operatorname{Re}\{\langle f, \mathcal{S}_\zeta^*(\bar{\lambda}) \rangle\},
 \end{aligned}$$

and consequently, $\mathcal{S}_\zeta^*(\bar{\lambda}) = \int_0^1 \left(\overline{\lambda(t)} \overline{K_1(\zeta(t), \zeta(s))} - \lambda(t) K_2(\zeta(t), \zeta(s)) \right) dt$.

B Derivatives of $K_1(\zeta, \tau)$ and $K_2(\zeta, \tau)$

This section presents the derivatives of the kernels $K_1(\zeta, \tau)$ and $K_2(\zeta, \tau)$ entering the gradient expression.

$$\begin{aligned}
\frac{\partial K_1(\zeta, \tau)}{\partial r} &= \frac{1}{\pi i} \left(\left[\frac{z_1 - z}{2(\tau - \zeta)^2} - \frac{C_1(\zeta, \tau)}{2r} \right] \Omega_+^{(0)}(\zeta, \tau) + \frac{r_1^2 - r^2 + (z - z_1)^2}{2r |\zeta + \bar{\tau}|^2} C_1(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau) \right), \\
\frac{\partial K_1(\zeta, \tau)}{\partial r_1} &= \frac{1}{\pi i} \left(\left[\frac{z - z_1}{2(\tau - \zeta)^2} + \frac{C_1(\zeta, \tau)}{2r_1} \right] \Omega_+^{(0)}(\zeta, \tau) + \frac{r^2 - r_1^2 + (z - z_1)^2}{2r_1 |\zeta + \bar{\tau}|^2} C_1(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau) \right), \\
\frac{\partial K_2(\zeta, \tau)}{\partial r} &= \frac{1}{\pi i} \left(\left[\frac{z - z_1}{2(\zeta + \bar{\tau})^2} - \frac{C_2(\zeta, \tau)}{2r} \right] \Omega_-^{(0)}(\zeta, \tau) + \frac{r_1^2 - r^2 + (z - z_1)^2}{2r |\zeta - \tau|^2} C_2(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau) \right), \\
\frac{\partial K_2(\zeta, \tau)}{\partial r_1} &= \frac{1}{\pi i} \left(\left[\frac{z - z_1}{2(\zeta + \bar{\tau})^2} + \frac{C_2(\zeta, \tau)}{2r_1} \right] \Omega_-^{(0)}(\zeta, \tau) + \frac{r^2 - r_1^2 + (z - z_1)^2}{2r_1 |\zeta - \tau|^2} C_2(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau) \right), \\
\frac{\partial K_1(\zeta, \tau)}{\partial z} &= \frac{1}{\pi i} \left(\frac{r - r_1}{2(\tau - \zeta)^2} \Omega_+^{(0)}(\zeta, \tau) - \frac{z - z_1}{|\zeta + \bar{\tau}|^2} C_1(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau) \right), \\
\frac{\partial K_2(\zeta, \tau)}{\partial z} &= -\frac{1}{\pi i} \left(\frac{r + r_1}{2(\zeta + \bar{\tau})^2} \Omega_-^{(0)}(\zeta, \tau) + \frac{z - z_1}{|\zeta - \tau|^2} C_2(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau) \right), \\
\frac{\partial K_1(\zeta, \tau)}{\partial z_1} &= -\frac{\partial K_1(\zeta, \tau)}{\partial z}, \quad \frac{\partial K_2(\zeta, \tau)}{\partial z_1} = -\frac{\partial K_2(\zeta, \tau)}{\partial z}.
\end{aligned}$$

C Derivatives of the Kernels for Transversal Motion

This section presents the derivatives of the kernels $M_1(\zeta, \tau)$, $M_2(\zeta, \tau)$, $M_3(\zeta, \tau)$ and $M_4(\zeta, \tau)$ entering the gradient expression for transversal translation of the body of revolution.

$$\begin{aligned}
\frac{\partial M_1(\zeta, \tau)}{\partial r} &= \frac{1}{\pi i} \left(\frac{z_1 - z}{(\tau - \zeta)^2} - \frac{1}{2r} C_{11}(\zeta, \tau) \right) \Omega_+^{(0)}(\zeta, \tau) + \frac{1}{\pi i} \frac{r_1^2 - r^2 + (z - z_1)^2}{2r |\zeta + \bar{\tau}|^2} C_{11}(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau), \\
\frac{\partial M_1(\zeta, \tau)}{\partial r_1} &= \frac{1}{\pi i} \left(\frac{z - z_1}{(\tau - \zeta)^2} + \frac{1}{2r_1} C_{11}(\zeta, \tau) \right) \Omega_+^{(0)}(\zeta, \tau) + \frac{1}{\pi i} \frac{r^2 - r_1^2 + (z - z_1)^2}{2r_1 |\zeta + \bar{\tau}|^2} C_{11}(\zeta, \tau) \Omega_-^{(0)}(\zeta, \tau), \\
\frac{\partial M_1(\zeta, \tau)}{\partial z} &= \frac{1}{\pi i} \frac{r - r_1}{(\tau - \zeta)^2} \Omega_+^{(0)}(\zeta, \tau) - \frac{1}{\pi i} C_{11}(\zeta, \tau) \frac{z - z_1}{|\zeta + \bar{\tau}|^2} \Omega_-^{(0)}(\zeta, \tau), \\
\frac{\partial M_1(\zeta, \tau)}{\partial z_1} &= -\frac{\partial M_1(\zeta, \tau)}{\partial z}, \\
\frac{\partial M_2(\zeta, \tau)}{\partial r} &= \frac{1}{\pi i} \left(\frac{z - z_1}{(\bar{\tau} + \zeta)^2} - \frac{1}{2r} C_{21}(\zeta, \tau) \right) \Omega_-^{(0)}(\zeta, \tau) + \frac{1}{\pi i} \frac{r_1^2 - r^2 + (z - z_1)^2}{2r |\zeta - \tau|^2} C_{21}(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau), \\
\frac{\partial M_2(\zeta, \tau)}{\partial r_1} &= \frac{1}{\pi i} \left(\frac{z - z_1}{(\bar{\tau} + \zeta)^2} + \frac{1}{2r_1} C_{21}(\zeta, \tau) \right) \Omega_-^{(0)}(\zeta, \tau) + \frac{1}{\pi i} \frac{r^2 - r_1^2 + (z - z_1)^2}{2r_1 |\zeta - \tau|^2} C_{21}(\zeta, \tau) \Omega_+^{(0)}(\zeta, \tau), \\
\frac{\partial M_2(\zeta, \tau)}{\partial z} &= -\frac{1}{\pi i} \frac{r + r_1}{(\bar{\tau} + \zeta)^2} \Omega_-^{(0)}(\zeta, \tau) - \frac{1}{\pi i} C_{21}(\zeta, \tau) \frac{z - z_1}{|\zeta - \tau|^2} \Omega_+^{(0)}(\zeta, \tau),
\end{aligned}$$

$$\frac{\partial M_2(\zeta, \tau)}{\partial z_1} = -\frac{\partial M_2(\zeta, \tau)}{\partial z},$$

$$\frac{\partial M_3(\zeta, \tau)}{\partial r} = \frac{1}{\pi i} \left(\frac{r_1^2 - r^2 + (z - z_1)^2}{\tau - \zeta} \frac{\Omega_-^{(0)}(\zeta, \tau) - 3\Omega_-^{(1)}(\zeta, \tau)}{2r|\zeta + \bar{\tau}|^2} - \frac{\tau - \zeta - 2r}{2r(\tau - \zeta)^2} \left(\Omega_+^{(0)}(\zeta, \tau) - \Omega_+^{(1)}(\zeta, \tau) \right) \right),$$

$$\frac{\partial M_3(\zeta, \tau)}{\partial r_1} = \frac{1}{\pi i} \left(\frac{r^2 - r_1^2 + (z - z_1)^2}{\tau - \zeta} \frac{\Omega_-^{(0)}(\zeta, \tau) - 3\Omega_-^{(1)}(\zeta, \tau)}{2r_1|\zeta + \bar{\tau}|^2} + \frac{\tau - \zeta - 2r_1}{2r_1(\tau - \zeta)^2} \left(\Omega_+^{(0)}(\zeta, \tau) - \Omega_+^{(1)}(\zeta, \tau) \right) \right),$$

$$\frac{\partial M_3(\zeta, \tau)}{\partial z} = \frac{1}{\pi i} \frac{z_1 - z}{\tau - \zeta} \frac{\Omega_-^{(0)}(\zeta, \tau) - 3\Omega_-^{(1)}(\zeta, \tau)}{|\zeta + \bar{\tau}|^2} + \frac{1}{\pi} \frac{\Omega_+^{(0)}(\zeta, \tau) - \Omega_+^{(1)}(\zeta, \tau)}{(\tau - \zeta)^2},$$

$$\frac{\partial M_3(\zeta, \tau)}{\partial z_1} = -\frac{\partial M_3(\zeta, \tau)}{\partial z},$$

$$\frac{\partial M_4(\zeta, \tau)}{\partial r} = \frac{1}{\pi i} \left(\frac{r_1^2 - r^2 + (z - z_1)^2}{|\zeta - \tau|^2} \frac{\Omega_+^{(0)}(\zeta, \tau) + 3\Omega_+^{(1)}(\zeta, \tau)}{2r(\bar{\tau} + \zeta)} - \frac{\bar{\tau} + \zeta + 2r}{2r(\bar{\tau} + \zeta)^2} \left(\Omega_-^{(0)}(\zeta, \tau) + \Omega_-^{(1)}(\zeta, \tau) \right) \right),$$

$$\frac{\partial M_4(\zeta, \tau)}{\partial r_1} = \frac{1}{\pi i} \left(\frac{r^2 - r_1^2 + (z - z_1)^2}{|\zeta - \tau|^2} \frac{\Omega_+^{(0)}(\zeta, \tau) + 3\Omega_+^{(1)}(\zeta, \tau)}{2r_1(\bar{\tau} + \zeta)} + \frac{\bar{\tau} + \zeta - 2r_1}{2r_1(\bar{\tau} + \zeta)^2} \left(\Omega_-^{(0)}(\zeta, \tau) + \Omega_-^{(1)}(\zeta, \tau) \right) \right),$$

$$\frac{\partial M_4(\zeta, \tau)}{\partial z} = \frac{1}{\pi i} \frac{z_1 - z}{|\zeta - \tau|^2} \frac{\Omega_+^{(0)}(\zeta, \tau) + 3\Omega_+^{(1)}(\zeta, \tau)}{\bar{\tau} + \zeta} - \frac{1}{\pi} \frac{\Omega_-^{(0)}(\zeta, \tau) + \Omega_-^{(1)}(\zeta, \tau)}{(\bar{\tau} + \zeta)^2},$$

$$\frac{\partial M_4(\zeta, \tau)}{\partial z_1} = -\frac{\partial M_4(\zeta, \tau)}{\partial z},$$

$$\frac{\partial}{\partial r} \left(\frac{\Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = \frac{1}{\tau - \zeta} \left(3 \frac{r_1^2 - r^2 + (z - z_1)^2}{2r|\zeta + \bar{\tau}|^2} \Omega_-^{(1)}(\zeta, \tau) + \frac{2r - \tau + \zeta}{2r(\tau - \zeta)} \Omega_+^{(1)}(\zeta, \tau) \right),$$

$$\frac{\partial}{\partial r_1} \left(\frac{\Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = \frac{1}{\tau - \zeta} \left(3 \frac{r^2 - r_1^2 + (z - z_1)^2}{2r_1|\zeta + \bar{\tau}|^2} \Omega_-^{(1)}(\zeta, \tau) + \frac{\tau - \zeta - 2r_1}{2r_1(\tau - \zeta)} \Omega_+^{(1)}(\zeta, \tau) \right),$$

$$\frac{\partial}{\partial z} \left(\frac{\Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = \frac{1}{\tau - \zeta} \left(3 \frac{z_1 - z}{|\zeta + \bar{\tau}|^2} \Omega_-^{(1)}(\zeta, \tau) + \frac{i \Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta} \right),$$

$$\frac{\partial}{\partial z_1} \left(\frac{\Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = -\frac{\partial}{\partial z} \left(\frac{\Omega_+^{(1)}(\zeta, \tau)}{\tau - \zeta} \right),$$

$$\frac{\partial}{\partial r} \left(\frac{\Omega_-^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = \frac{1}{\bar{\tau} + \zeta} \left(3 \frac{r_1^2 - r^2 + (z - z_1)^2}{2r|\zeta - \tau|^2} \Omega_+^{(1)}(\zeta, \tau) - \frac{\bar{\tau} + \zeta + 2r}{2r(\bar{\tau} + \zeta)} \Omega_-^{(1)}(\zeta, \tau) \right),$$

$$\frac{\partial}{\partial r_1} \left(\frac{\Omega_-^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = \frac{1}{\bar{\tau} + \zeta} \left(3 \frac{r^2 - r_1^2 + (z - z_1)^2}{2r_1|\zeta - \tau|^2} \Omega_+^{(1)}(\zeta, \tau) + \frac{\bar{\tau} + \zeta - 2r_1}{2r_1(\bar{\tau} + \zeta)} \Omega_-^{(1)}(\zeta, \tau) \right),$$

$$\frac{\partial}{\partial z} \left(\frac{\Omega_-^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = \frac{1}{\bar{\tau} + \zeta} \left(3 \frac{z_1 - z}{|\zeta - \tau|^2} \Omega_+^{(1)}(\zeta, \tau) - \frac{i \Omega_-^{(1)}(\zeta, \tau)}{\bar{\tau} + \zeta} \right),$$

$$\frac{\partial}{\partial z_1} \left(\frac{\Omega_-^{(1)}(\zeta, \tau)}{\tau - \zeta} \right) = -\frac{\partial}{\partial z} \left(\frac{\Omega_-^{(1)}(\zeta, \tau)}{\tau - \zeta} \right).$$

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