Solution to shape optimization problems of viscous flow fields

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This paper presents a numerical solution to the shape optimization problems of steady-state viscous flow fields. The minimization problem of total dissipation energy was formulated in the domain of viscous flow fields. The shape gradient of the shape optimization problem was derived theoretically using the adjoint variable method, the Lagrange multiplier method and the formulae of the material derivative. Reshaping was carried out by the traction method proposed by one of the authors as an approach to solving domain optimization problems. The validity of the proposed method was confirmed by results of 2D and 3D numerical analyses.

Keywords: Shape optimization; Optimum design; Computational fluid dynamics; Finite-element method; Shape gradient; Adjoint variable method

1. Introduction

Shape determination problems in which the drag-power of a moving body in a viscous fluid or total dissipation energy in a channel for transportation of viscous fluid is minimized are important problems in engineering from the viewpoint of increasing energy efficiency.

Shape optimization theory of incompressible viscous flow fields was initiated by Pironneau (1973, 1974, 1984). He formulated a shape optimization problem of an isolated body located in a uniform viscous flow field to minimize drag-power and derived the distributed shape sensitivity, which was called the shape gradient, with respect to domain variation by means of an adjoint variable method based on optimal control theory. The adjoint variable method introduces adjoint variables into variational forms of state equations as variational variables and determines the adjoint variables using adjoint equations derived under the criteria of an optimality condition with respect to domain variation. In the viscous flow field problem, the analysis of an adjoint flow velocity and an adjoint pressure is required by adjoint equations in addition to the state equations, i.e. the Navier–Stokes equation and the continuity equation for the flow velocity and the pressure.

In subsequent work, Glowinski and Pironneau (1975) presented numerical solutions of the minimum-drag profile of a 2D body located in laminar flow using a boundary-layer splicing method, i.e. a inviscid/viscid patching method. Independently of that group, for many years Jameson (1988, 1995) also advocated and used control-theory techniques in the aerodynamic design of computational fluid dynamics using a continuous adjoint variable method.

Sano and Sakai (1983) and Ganesh (1994) analyzed 2D shape optimization problems of an isolated body for Stokes flow fields using the numerical procedure proposed by Pironneau (1984), in which degrees of freedom for finite element nodal points at the isolated body surface are chosen as design variables, and obtained an elliptic shape as the optimal shape. Also, Ganesh (1994) analyzed a similar problem at a Reynolds number of 20 and obtained an ovoid where the sharp end pointed to the upstream of the flow as the optimal shape. Huan and Modi (1994, 1996) analyzed similar isolated body problems at a high Reynolds number, where they solved original state equations and adjoint equations using modified boundary conditions, i.e. replacing the outflow Dirichlet conditions with less restrictive Neumann conditions for the boundary conditions of viscous flow fields.

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The numerical optimization procedure used in these works involved the use of a general-purpose program of mathematical programming, such as the steepest descent method, based on the shape sensitivity for the discrete model. These methods, however, present the disadvantage of the large computational calculation time required for optimization processing when the number of the degrees of freedom of the finite element model increases, and the mesh of internal nodes had to be refined in the process of updating the shape.

The authors have also addressed the solution of the shape optimization problem based on the gradient method using the shape gradient. In a previous study (Katamine and Azegami 1995), the authors presented a numerical analysis method for dissipation energy minimization problem of steady-state viscous flow fields and analyzed the 2D Stokes flow problems. Reshaping was accomplished by the traction method (Azegami 1994, 2000, Azegami et al., 1997), that was proposed as a solution to the boundary shape optimization problems of domains in which boundary value problems of partial differential equations are defined. In the traction method, domain variations that minimize the objective functional are obtained as solutions of pseudo-linear elastic problems of continua defined in the design domain and loaded with pseudo-distributed traction in proportion to the shape gradient in the design domain. Numerical solutions of both evaluation of the shape gradient and pseudo-linear elastic problems for evaluation of domain variation can be obtained using the finite-element method or the boundary-element method. Since the traction method is implemented by the use of the finite element method or boundary element method, it is exceptionally easy to perform and offers the advantage that it is not necessary to refine the mesh of the internal nodes of the domain.

In this paper, a dissipation energy minimization problem of viscous flow fields considering a convection term is dealt with. Based on the formulation of the shape optimization problem, the governing equations for calculating the shape gradient are derived using the adjoint variable method, the Lagrange multiplier method and the formulae of the material derivative. For reshaping, the traction method is employed. The finite element method is used to obtain the numerical solutions for the viscous flow fields analysis, adjoint equations and reshaping by the traction method. The validity of this numerical method is confirmed by several numerical results for 2D low-Reynolds-number viscous flow problems and 3D Stokes flow problems obtained using a general purpose FEM code.

2. Domain variation

Before formulating the shape optimization problem, a method of representing domain variation using the speed method will be discussed briefly. A more detailed explanation is given in Sokolowski and Zolésio (1992).

Suppose that a domain $\Omega \subset R^n$, where $n = 2, 3, R$ is the set of real numbers, and its boundary $\Gamma$, is variable. One approach to describing the domain variation is to use a one-parameter family of one-to-one mapping $T_s(X) : \Omega \ni X \mapsto x \in \Omega_s$, where $s$ denotes the domain variation history.

When a domain functional $J_\Omega$ of a distributed function $\phi$ is considered, its derivative $J_\Omega$ with respect to $s$ at $s = 0$ is given by the formulae of the material derivative:

$$J_\Omega = \int_\Omega \phi \, dx, \quad J_\Omega = \int_\Omega \phi' \, dx + \int_\Gamma \phi \nu \cdot V \, dx, \tag{1}$$

where $\nu$ is an outward unit normal vector on the boundary. The shape derivative $\phi'$ of distributed function $\phi$ indicates the derivative under a spatially fixed condition. The derivative of $T_s(X)$ with respect to $s$ given by

$$V(x) = \frac{\partial T_s}{\partial s} (T_s^{-1}(X)), \quad X \in \Omega_s, \quad x \in \Omega, \tag{2}$$

is called the velocity because of the analogy between $s$ and time.

3. Total dissipation energy minimization problem of viscous flow field

Let us consider a steady-state viscous flow field of an incompressible Newtonian fluid on domain $\Omega \subset R^n$ with the boundaries $\Gamma = \Gamma_0 \cup \Gamma_w \cup \Gamma_1$. Let flow velocity $u = \{u_i\}_{i=1}^n \in U$ be bounded with a prescribed flow velocity $\bar{u} \in (H^{1/2}(\Omega))^n$ on non-homogeneous Dirichlet-type sub-boundary $\Gamma_0$ and $u = 0$ on homogeneous Dirichlet-type sub-boundary $\Gamma_w$.

$$U = \{u \in (H^1(\Omega))^n | u = \bar{u} \text{ on } \Gamma_0, \quad u = 0 \text{ on } \Gamma_w \} \tag{3}$$

and satisfy

$$\{ -p \delta_{ij} + \mu (u_{ij} + u_{ji}) \} v_j = \hat{\sigma}_i \text{ on } \Gamma_1 \tag{4}$$

with a prescribed force $\hat{\sigma} = \{\hat{\sigma}_i\}_{i=1}^n \in (H^{-1/2}(\Gamma_1))^n$ on Neumann-type subboundary $\Gamma_1$.

Let pressure $p \in Q$:

$$Q = \{q \in L^2(\Omega), \quad \int_\Omega q \, dx = 0 \tag{5}$$

(if means $\Gamma_1 = 0$).

Density $\rho \in L^\infty(\Omega)$ and viscosity coefficient $\mu \in L^\infty(\Omega)$ are assumed to be given.

3.1 Formulation of problem

The total dissipation energy minimization problem under volume constraint $M > 0$ is formulated as

Problem : \begin{align} \text{Given } M \text{ and } \hat{u}, \hat{\sigma}, p, \mu : \text{fixed in space,} \\
\text{find } \Omega \text{ that minimize } a^V(u, u) \tag{6} \\
\text{subject to } a^V(u, w) + b(u, u, w) - c(w, p) = d(w) \tag{9} \end{align}
\[ c(u, q) = 0 \quad \forall q \in Q \quad (10) \]
\[
\int_{\Omega} \, dx \leq M, \quad (11)
\]
where equations (9) and (10) are variational forms, or weak forms, using the adjoint velocity \( w = \{ w_i \}_{i=1}^{n} \in W : \)
\[
W = \{ w \in (H^1(\Omega))^n | w = 0 \text{ on } \Gamma_0 \cup \Gamma_w \} \quad (12)
\]
and the adjoint pressure \( q \in Q \) for the state equations, i.e., the Navier–Stokes equation and continuity equation. Equation (11) gives the constraint with respect to volume. The viscous term \( a^V(u, w) \), the convective term \( b(v, u, w) \), the pressure term \( c(w, p) \), and the stress term \( d(w) \) are defined as
\[
a^V(u, w) = \int_{\Omega} 2\mu e_{ij}(u) e_{ij}(w) \, dx = \int_{\Omega} \mu w_i, j(u_i + u_j) \, dx, \\
b(v, u, w) = \int_{\Omega} \rho w_i v_j u_{ij} \, dx, \\
c(w, p) = \int_{\Omega} w_i, p \, dx, \\
d(w) = \int_{\Gamma_1} w_i \delta_i \, d\Gamma,
\]
where \( e_{ij}(u) = 1/2(u_{ij} + u_{ji}) \). The Einstein summation convention and partial differential notation \( \partial_i = \partial/\partial x_i \) are used in the tensor notation of this paper.

### 3.2 Shape gradient

Applying the concept of the Lagrange multiplier method and adjoint variable method, this problem can be rendered into a stationary problem of the Lagrange functional \( L(u, p, w, q) \),
\[
L = a^V(u, u) - a^V(u, w) - b(u, u, w) + c(w, p) + d(w) + c(u, q) + \Lambda \left( \int_{\Omega} dx - M \right), \quad (13)
\]
where \( w \in W \) and \( q \in Q \) are the adjoint variables with respect to the flow velocity and the pressure, respectively. The non-negative real number \( \Lambda \) is the Lagrange multiplier with respect to the volume constraint.

For simplicity, when assuming that the non-homogeneous Dirichlet-type sub-boundary \( \Gamma_0 \) and the Neumann-type sub-boundary \( \Gamma_1 \) are invariable under reshaping, the derivative \( \tilde{L} \) with respect to \( s \) is derived using the formulae of equation (1):
\[
\tilde{L} = \{ a^V(u, w') + b(u, u, w') - c(w', p) - d(w') \} \\
+ c(u, q') - \{ a^V(u', w) + b(u', u, w) \} \\
+ b(u, u', w) - c(u', q) - 2a^V(u, u') \\
+ c(w, p') + \Lambda \left( \int_{\Omega} dx - M \right) + \langle Gv, V \rangle, \quad (14)
\]
where \( (\cdot) \) is the material derivative, and \( (\cdot') \) is the shape derivative for the domain variation of the distributed function under a spatially fixed condition. The linear form \( \langle Gv, V \rangle \) with respect to the velocity function \( V \) is given by
\[
\langle Gv, V \rangle = \int_{\Gamma_0} G_v V_d \, d\Gamma \quad (15)
\]
\[
G = \mu u_i, j(u_i + u_j) - \mu w_i, j(u_i + u_j) + \Lambda. \quad (16)
\]
Considering stationary conditions for all \( w' \in W, q' \in Q, u' \in W \) and \( p' \in Q \) from equation (14), the Kuhn–Tucker conditions with respect to \( u, p, w, q \) are obtained as
\[
a^V(u, w') + b(u, u, w') - c(w', p) = d(w') \\
\forall w' \in W \]
\[
c(u, q') = 0 \quad \forall q' \in Q \quad (18)
\]
\[
a^V(u', w) + b(u', u, w) + b(u, u', w) \\
- c(u', q) - 2a^V(u, u') = 0 \quad \forall u' \in W \quad (19)
\]
\[
c(w, p') = 0 \quad \forall p' \in Q \quad (20)
\]
\[
\Lambda \geq 0, \quad \int_{\Omega} dx \leq M, \quad \Lambda \left( \int_{\Omega} dx - M \right) = 0, \quad (21)
\]
that indicate variational forms of the original state equations for flow velocity \( u \) and pressure \( p \), variational forms of the adjoint equations for adjoint velocity \( w \), and adjoint pressure \( q \), respectively, which we call adjoint equations. Under the condition satisfying equations (17)–(21), the derivative of the Lagrange functional agrees with that of the objective functional and the linear form \( \langle Gv, V \rangle \) with respect to the velocity function \( V \):
\[
\tilde{L}|_{u, p, w, q, \Lambda} = \langle Gv, V \rangle. \quad (22)
\]

The coefficient vector \( Gv \) in equation (15) has the meaning of a sensitivity relation to domain variation and is called a shape gradient. Scalar function \( G \) is called the shape gradient density.

### 4. Numerical solution technique

#### 4.1 Traction method

When the shape gradient is obtained, the traction method (Azegami 1994, 2000, Azegami et al., 1997) can be applied to optimize the geometrical domain shape. The traction method has been proposed as a procedure for solving the velocity \( V \in D \) by
\[
a^F(V, y) = -\langle Gv, y \rangle, \quad \forall y \in D, \quad (23)
\]
where \( a^F(\cdot, \cdot) \) is defined by
\[
a^F(u, v) = \int_{\Omega} A_{ijkl} u_k v_{ij} \, dx \quad (24)
\]
\( D = \{ V \in (H^1(\Omega))^n \mid \text{constraints of domain variation} \}, \)

(25)

where \( u = \{ u_i \}_{i=1}^n, \ v = \{ v_i \}_{i=1}^n \) and \( \{ A_{ijkl} \}_{i,j,k,l=1,2,...,n} \) are displacement, variational displacements and an elastic tensor, respectively. Equation (23) indicates that the velocity \( V \) decreasing the objective functional, that is the dissipation energy in this study, is obtained as a displacement of a pseudo-elastic body defined in \( \Omega \) by the loading of a pseudo-external force in proportion to \( 2Gn \), under constraints on the displacement of invariable boundaries.

### 4.2 Numerical procedure

A flow chart of the shape optimization system is shown in figure 1. The finite element method was employed in every analysis. Shape optimization analysis was performed by executing these elements sequentially and repeatedly.

The shape gradient was evaluated using the two viscous flow field analyses which analyze distributions of flow velocity \( u \), pressure \( p \) for the non-linear original state equations (17) and (18) and the distributions of adjoint flow velocity \( w \), and adjoint pressure \( q \) for the linear adjoint equations (19) and (20).

The shape gradient was calculated using the results. Domain variation \( V \) in equation (23) was analyzed using the finite element method, with the second order finite element for \( V \). The Lagrange multiplier \( \Lambda \), determined so as to satisfy the volume constraint, can be regarded as a uniform surface force in external force \(-Gn\). Therefore, it should be possible to satisfy the conditions of equation (21) by controlling the magnitude of this uniform surface force \( \Lambda \).

### 5. Numerical results

#### 5.1 2D low-Reynolds-number problems

We present numerical results of 2D low-Reynolds-number viscous flow problems of an isolated body in uniform flow and a branch channel, as shown in figures 2 and 3.

In figure 2, the FEM model and boundary condition for the isolated body problem are shown, and the design boundary was assumed on the surface boundary \( \Gamma_w \) of the isolated body. The Reynolds number is defined from the magnitude of uniform flow \( \hat{u} \) and the initial diameter of an isolated body. Figure 4 shows the results of the isolated body problem. These results show comparisons of flow velocity \( u \), pressure \( p \), adjoint flow velocity \( w \) for initial shape, and converged shapes between \( Re = 0.1 \) (Stokes flow) and \( Re = 40 \). On the basis of these results, we can observe that the optimal shape is the ellipse at the Stokes flow and the ovoid where the sharp end points to the upstream of the flow at \( Re = 40 \). This numerical result for
Stokes flow is in good agreement with the shape analyzed by Sano and Sakai (1983) and Ganesh (1994). Moreover, in the case of a Stokes flow problem, we can confirm that the magnitude of the adjoint flow velocity $w$ is very small compared with that of the usual flow velocity $u$, so it could be neglected. Monotonic convergences of iteration histories of dissipation energy in both problems confirm the validity of the proposed method.

In figure 3 for the branch channel problem, fluid flows in from a boundary $G_0$ and flows out from two boundaries $G_1$. Poiseulle flow $\hat{u}$ was assumed at the entrance boundary $G_0$, and prescribed force $\hat{\sigma} = 0$ was assumed at the exit boundaries $G_1$. The design boundary was assumed on the whole wall boundary $G_w$. The Reynolds number is defined from the mean of Poiseulle flow $\hat{u}$ and the width at entrance boundary $G_0$. The numerical results of this problem at $Re = 0.1$ (Stokes flow) and $Re = 100$ are shown in figure 5, in the same manner as the results of isolated body problem. The values of the objective functional in both problems were converged, and thus we confirmed the validity of the present method.

5.2 3D Stokes flow problems using a general-purpose FEM program

In this study, if we assume a Stokes flow problem in which we can neglect the effect of a convective term, the shape gradient density $G$ is equivalent to the dissipation energy density $\mu u_{ij}(u_{ij} + u_{ji})$. On the basis of the actual numerical results for Stokes flow shown in figures 4 and 5, we confirmed that the effect for the distribution of adjoint velocity $w$ can be neglected, and therefore we do not need to solve the adjoint equations (19) and (20) for the adjoint velocity $w$ and adjoint pressure $q$.

A new general-purpose FEM system using ANSYS was developed for the shape optimization in the Stokes flow problems. The shape gradient was evaluated using a viscous flow analysis code in ANSYS/FLOTRAN. The domain variation $V$ was analyzed using a structural analysis code in ANSYS. Shape optimization analysis was performed by repeatedly executing these elements sequentially.

To confirm the validity of the developed system, the 3D problems of an isolated body and a branch channel for Stokes flow were analyzed. Figure 6 shows these problems. For both problems, Poiseulle flow $\hat{u}$ was assumed at entrance boundary $G_0$, and the prescribed force $\hat{\sigma} = 0$ was assumed at exit boundaries $G_1$. In the isolated body problem, the quarter-symmetricity was used. Figures 7 and 8 shows comparison of the meshes and distribution of the shape gradient $G$ between the initial shape and the converged shape. We can see that the distributions of shape gradient $G$ on the design boundary were uniform at each converged shape in figures 7 and 8. From the results...
of the isolated body problem, we can observe that the initial spherical ball shape changes into a rugby ball shape. The values of the objective functional decreased 1.4% for the isolated body problem and 9.0% for the branch channel problem.

According to the numerical results of these basic problems, we confirmed the validity of the present method.

Figure 5. Results of flow field analyses, converged shapes and iterative histories of dissipation energy in a branch problem.

Figure 6. 3D problems and finite element meshes.

Figure 7. Results of meshes and distributions of shape gradient near isolated body in the 3D isolated body problem.

Figure 8. Results of meshes and distributions of shape gradient in the 3D branch problem.
6. Conclusions

In this paper, we formulated a dissipation energy minimization problem for steady-state viscous flow fields and derived the shape gradient with respect to the problem. The validity of the traction method using the derived shape gradient was confirmed on the basis of the results of 2D and 3D numerical analyses.

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