Shape optimization problem based on the generalized J integral considering RANS and Snapshot POD

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Abstract
For suppression of time periodic flow and normal stress using optimal design techniques, this paper presents an optimal shape by sensitivity based on the Generalized J Integral, and makes a comparison to results of sensitivity evaluated by boundary and volume integrations of a type that is widely used for shape optimization problems. To date, J integral has been used to evaluate the energy release rate of stress concentrated near cracks or corners in the field of fracture mechanics. The Generalized J integration type used for this study is sensitive to avoid singularity and to engender the suppression of stress concentration in the domain and at the boundary. For such shape optimization studied here, the cost function is defined as eigenvalues with modes of the time fluctuation component in Snapshot POD. The main problems are the Reynolds Average Navier–Stokes problem and eigenvalue problem of Snapshot POD. An objective functional is described using Lagrange multipliers and finite element method. The sensitivity is obtained in three kinds of ways, the boundary and volume, the Generalized J integration types. Numerical results reveal that the cost function is minimized as the time periodic flow is suppressed in such the three ways. Especially, normal stress on the boundary in the sensitivity evaluated by the Generalized J integration type is suppressed most of them.

Keywords: Adjoint method, Cavity flow, Shape optimization problem, Snapshot proper orthogonal decomposition

1. Introduction
This paper presents a solution to a shape optimization problem constructed for suppressing not only a time periodic flow and but also normal stress on the boundary. Recently, Nakazawa (2018) specifically examined construction of a shape optimization method to suppress a time periodic flow at a sufficiently low Reynolds number based on Snapshot Proper Orthogonal Decomposition (Snapshot POD). However, Nakazawa (2018) considered the Time Average Navier–Stokes equation (TANS) as a main problem. Therefore, Reynolds Average Navier–Stokes equation (RANS) was not used. Additionally, sensitivity was evaluated by the boundary integration type (more details are available in eq. (38) of Appendix 7.1 ) used widely in the field of the shape optimization problems, and which is not guaranteed mathematical regularity for a boundary where a crack or corner appears. Therefore, it is unclear that the cost function is decreasing sufficiently to take its minimum value. Thereby, RANS is chosen for this study as the main problem instead of TANS. Also, sensitivities evaluated by the volume and the Generalized J integration types are used. Especially, the volume integration type and the Generalized J integration type (more details are available in eq. (40) of Appendix 7.1) are able to guarantee mathematical regularity only in the domain and both of in the domain and on the boundary. By the way, in recent years, fluid machinery like car is designed by topology optimization shown in Othmer (2014). However, this paper uses shape optimization problem without using topology optimization, because the author wants
to consider fluid behavior near boundary. The particular history, background, and procedure of the suggested shape optimization problem are described below.

With the rapid development of computer technology and corresponding numerical methods for high-performance computing, the shape optimization scheme based on Computational Fluid Dynamics (CFD) always plays quite important roles in fluid mechanics and aerodynamic design. A classical shape optimization problem in fluid dynamics was first developed by Pironneau (1973, 1974) for domains in which the stationary Stokes and Navier-Stokes equations are defined, respectively. Subsequently, Haslinger and Makinen (2003), Mohammadi and Pironneau (2001), and Moubachir and Zolesio (2006) have been keeping constructions and developing fundamental frameworks of flow field shape optimization problems. Recently, many researchers are studying them. Based on the research background presented above, the original motivation of this paper can be described as presented below.

Although flow stabilization presents an important challenge that confronts the research field of flow control today, few reports of the relevant literature describe flow stabilization by shape optimization. For example, there are many literatures where the cost functions like lift coefficient and drag coefficient and so on are defined by the time average flow field. Nakazawa (2016) reported that minimization and maximization problems of dissipation energy are solved in the two-dimensional cavity flow, where the stationary Navier–Stokes problem is used as the main problem and dissipation energy is used as the cost function. After shape optimization, linear stability analysis is applied in the initial and the optimal domains. The critical Reynolds numbers are, respectively, decreasing and increasing. Next, to control the flow stability more directly, Nakazawa and Azegami (2015) reported a pioneering shape optimization method to stabilize the disturbances. The method is based on linear stability theory. Particularly, the real part of the leading eigenvalue is used as the cost function. To obtain the cost function, the stationary Navier–Stokes problem and the eigenvalue problem of the linear stability analysis are defined as the main problems. However, the methods explained above are not available for the case in which the non-stationary boundary condition is defined because the stationary Navier–Stokes problem should be solved to prepare a stationary solution for linear stability analysis. To address the challenge explained above, the author constructed a new shape optimization method (Nakazawa, 2018) using Snapshot Proper Orthogonal Decomposition (Snapshot POD). This Snapshot POD can decompose the time-dependent flow into a time average component and a time fluctuation component as orthogonal modes in the time direction. Such a methodology is the same as Primary Component Analysis (PCA). For such a shape optimization framework, the eigenvalue describing modes of the time fluctuation component in Snapshot POD can be defined as a cost function. A remarkable feature of this suggested shape optimization problem is that a time periodic flow driven only by the non-stationary boundary condition at a sufficiently low Reynolds number might be developed or suppressed efficiently because the eigenvalue (cost function) in Snapshot POD shows the $L^2$ norm of the velocity vector which takes the time average or the time fluctuation obtained by decomposing the time periodic flow into each orthogonal mode. A brief summary of the shape optimization problem addressed in this paper is presented below.

The sum of eigenvalues in the modes of the time fluctuation component in Snapshot POD is defined as the cost function. The Reynolds Average Navier–Stokes problem and the eigenvalue problem in POD are used as the main problems. The main problems are transformed from strong forms to weak forms with trial functions based on a standard application of finite element method (FEM). The functional is described using Lagrange multiplier method with FEM. Next, using adjoint variable method, its first variation (which is the same as the material derivative) is derived to evaluate sensitivity based on the Generalized J Integral. An initial domain is reshaped iteratively to obtain an optimal domain. Then the $H^1$ gradient method constructed by Azegami and Wu (1996) is used for stable domain deformation. Additionally, this paper uses Adaptive Mesh Refinement (AMR) after the mesh is reshaped by sensitivity, where the new mesh is generated with respect to the metric as constructed by Castro-Diaz and Hecht (2006) and by Alauzet et al. (2006).

In fact, throughout reshaping steps or in the case of initial domain with a crack and corner on the boundary, the stress concentration is known to appear on such a boundary. To date, the energy release rate is evaluated as the sensitivity in a cracked domain and which plays an important role in the field of fracture mechanics. The application of sensitivity to the energy release rate was studied originally as the Generalized J Integral in a series of works by Ohtsuka (1981, 1985, 1985), Ohtsuka and Khludnev (2000), and Ohtsuka and Khludnev (2018). Mathematical justification of the existence and derivation of some formulas in a general geometric situation were
conducted there. The sensitivity used for this study is evaluated based on the Generalized J integral.

For numerical demonstrations with FreeFEM++ (Hecht, 2012) for all numerical calculations, the same problem is taken over numerically as described below. Two-dimensional cavity flow with a disk-shaped isolated body is adopted, where the non-stationary boundary condition is defined on the top boundary and non-slip boundary condition for the boundaries not only of the side and bottom, but also of the disk. The disk boundary is used as the design boundary. Therefore, the disk is reshaped by the shape optimization process as the cost function decreases, where the domain variation is obtained from sensitivity analysis and where some cost functions combining eigenvalues with various primary components are introduced. After numerical calculations, the eigenvalues of Snapshot POD are compared in the initial domain and in the optimal domain. The effectiveness of the suggested shape optimization problem with AMR is confirmed. See mathematical aspects and specific details of such optimization problems in Appendix 7.6.

2. Problem Formulation

2.1. Initial domain

Let $\Omega_0$ be a fixed bounded Lipschitz domain in $\mathbb{R}^d$ ($d \in \mathbb{N}$). Additionally, let $\Omega$ be an open subset of $\Omega_0$, where a position vector is denoted as $x \in \mathbb{R}^d$. As described herein, the two-dimensional cavity flow with a disk-shaped isolated body $\Omega$ is adopted for the initial domain shown in Fig. 1. For $d = 2$, the initial domain is $\Omega \subset \Omega_0 \subset \mathbb{R}^2$,

$$\Omega = \Omega_M \setminus \Omega_m,$$  

$$\Omega_M = \{(x,y) ; 0 \leq x \leq 1, 0 \leq y \leq 1\},$$  

$$\Omega_m = \{(x,y) ; (x - 0.5)^2 + (y - 0.5)^2 \leq 0.1\},$$

regarding the boundary as

$$\Gamma_{\text{top}} = \{(x,y) ; 0 \leq x \leq 1, y = 1\},$$  

$$\Gamma_{\text{wall}} = \partial \Omega_M \setminus \Gamma_{\text{top}}.$$  

For domain reshaping, the disk boundary $\partial \Omega_m$ is used as the design boundary.

![Finite element meshes in the initial domain.](image)

2.2. Main problems

For a shape optimization problem considering Snapshot POD, the paper is concerned with main problems, which are the Reynolds Average Navier–Stokes problem, and the eigenvalue problem in Snapshot POD. For the problem considered below, it is assumed that an initial domain $\Omega$ and the boundaries are determined, and that the flow of a viscous incompressible fluid that occupies a bounded domain $\Omega$ in $\mathbb{R}^d$ is studied, and that the mapping $\phi$ of the position vector $x$ from the initial domain $\Omega$ to the optimal domain $\phi(\Omega)$ is given. Additional details related to mapping $\phi$ and its domain variation are available in the Appendix 7.1. The velocity $u$ and pressure $p$ are assumed to be satisfied in this domain $\Omega$. The Reynolds number $Re$ is defined with reference length $|\Gamma_{\text{top}}|$ and the reference speed, which is the maximum value in the $x$-direction velocity component on $\Gamma_{\text{top}}$.

2.3. Non-stationary Navier–Stokes problem

As described in this paper, the first non-stationary Navier–Stokes problem is prepared before deriving the Reynolds Average Navier–Stokes problem.
2.4. Snapshot proper orthogonal decomposition

Next, we define a snapshot proper orthogonal decomposition (Snapshot POD) analysis from time $t = T_1$ to $T_2$. The POD basis and eigenvalues obtained here are used to derive the Reynolds Average Navier–Stokes problem.

The correlation coefficient matrix $R \in \mathbb{R}^{m \times m}$ is formed as

$$\hat{u} = [u_1^N, \ldots, u_N^N] \in \mathbb{R}^{d \times m}$$

as

$$R(N_1, N_2, \hat{u}, \hat{u}) = \int_{\Omega} \hat{u}^T \hat{u} d\Omega.$$ 

Let eigenvalues and eigenfunctions in POD be $\omega \in \mathbb{R}^m$ and $\Phi \in \mathbb{R}^{m \times m}$,

$$\omega = [\omega^1, \ldots, \omega^m], \quad \omega^i \in \mathbb{R},$$

$$\hat{u} = [\hat{u}^1, \ldots, \hat{u}^m], \quad \hat{u}^i \in \mathbb{R}^m,$$

$$\Phi = \hat{u} \hat{u}^T \omega^{-1} \in \mathbb{R}^{d \times m},$$

where $R(N_1, N_2, \hat{u}, \hat{u})$ is a positive-semidefinite matrix satisfying the eigenvalue $0 \leq \omega$, and where $\Phi^i$ depicts the POD basis for the $i$-th primary component as

$$\Phi = [\Phi^1, \ldots, \Phi^i, \ldots, \Phi^m] \in \mathbb{R}^{d \times m}.$$ 

Using the definitions, we define snapshot POD analysis as described below.

Problem 2 (Snapshot Proper Orthogonal Decomposition) Let the solution $u$ of Problem 1 be given with identify matrix $I \in \mathbb{R}^{m \times m}$. Find $\omega \in \mathbb{R}^m$ and $\Phi \in \mathbb{R}^{m \times m}$ for $N_1, N_2 \in \mathbb{N}$ such that

$$\omega I \hat{u} = R(N_1, N_2, \hat{u}, \hat{u}) \hat{u} = 0.$$ 

2.4.1. Reynolds Average Navier–Stokes problem As described in this paper, Problem 1 is rewritten by introducing Reynolds Decomposition for time-dependent flows $\{u^n, p^n\}_{n=1}^{N_2}$. Finally, the Reynolds Average Navier–Stokes problem is derived with time average velocity $\bar{u}$ and time fluctuation velocity $u^f = u^n - \bar{u}$ as follows:

Problem 3 (Reynolds Average Navier–Stokes Problem) Let $\mathbf{x} \in \Phi(\Omega)$, find $(\bar{u}, \bar{p}) : \Omega \rightarrow \mathbb{R}^d \times \mathbb{R}$ such that

$$\bar{u} \cdot \nabla \bar{u} + \frac{1}{Re} \int_{T_1}^{T_2} (\nabla \cdot C)^T dt = -\nabla \bar{p} + \frac{1}{Re} \Delta \bar{u} \quad \text{in } \Omega,$$

$$\nabla \cdot \bar{u} = 0 \quad \text{in } \Omega,$$

$$\bar{u} = 0 \quad \text{on } \partial \Omega,$$

for a tensor

$$C = \sum_{n=N_1}^{N_2} u_n^f u_n^f = \mathbb{E}(\mathbf{C}) \in \mathbb{R}^{d \times d}, \quad \int_{T_1}^{T_2} (\nabla \cdot C)^T dt = \nabla \cdot \mathbb{C}^T.$$
The tensor is rewritten with POD basis $\Phi$ and eigenvalue $\omega$ with one trigonometric identity as shown below:

$$
\hat{C} = \frac{\pi}{4} \Phi_\omega (\Phi_\omega^T)^T \in \mathbb{R}^{d \times d} = \frac{\pi}{4} \sum_{i=2}^{m} \Phi_i^T (\Phi_i^T)^T,
$$  \hspace{1cm} (17)

$$
\Phi_\omega = \sum_{i=2}^{m} \Phi_i \in \mathbb{R}^d,
$$  \hspace{1cm} (18)

$$
\Phi_\omega^T = \Phi_\omega = \{ \Phi^1 \omega, \ldots, \Phi^m \omega \} \in \mathbb{R}^{d \times m}.
$$  \hspace{1cm} (19)

Numerically the time average velocity $\bar{u}$ is estimated by $\Phi_i^T$. Additional details related to derivation of $\hat{C}$ are available in the Appendix 7.5.

3. Shape Optimization Problem

In this section, the shape optimization problem using Snapshot POD with weight function $\delta_{j \rightarrow k}$ is constructed. Next, based on the Kuhn–Tucker condition, the main and adjoint problems are solved to obtain the main and adjoint variables, which are substituted into the first variation to evaluate sensitivity for the shape optimization problem.

3.1. Lagrange function and its material derivative

We formulate the following a minimization problem of the cost function $f$ as

$$
f(\omega) = \sum_{i=1}^{m} \delta_{j \rightarrow k} \omega_i,
$$  \hspace{1cm} (20)

where $\delta_{j \rightarrow k}$ represents the weight function to extract $j$ to the $k$ primary components in $1$ to the $m$ primary components.

Problem 4 (Shape Optimization) After letting $f(\omega)$ be defined as Eq. (20), find $\phi(\Omega)$ such that

$$
\min_{\phi} \{ f(\omega) : \{(u^r, p^r)\}_{r=1}^{N_2}, (\omega, \hat{u}) \}. \hspace{1cm} (21)
$$

By application of the Lagrange multiplier method, Lagrange function $L$ for the shape optimization problem in this study is written as

$$
L(\Omega, \bar{\zeta}_1, \bar{\zeta}_2) = f(\omega) + L_1 (\Omega, \bar{\zeta}_1) + L_2 (\Omega, \bar{\zeta}_2), \hspace{1cm} (22)
$$

where the constraint function $L_2(\Omega, \bar{\zeta}_2)$ for Problem 2 with $\bar{\zeta}_2 = \{ \omega, \hat{u}, \alpha, u \}$ defined in Appendix 7.3 and $L_1(\Omega, \bar{\zeta}_1)$ for Problem 3 with $\bar{\zeta}_1 = \{ \bar{u}, \bar{\rho}, \bar{w}, \bar{q}, \bar{\Phi}_u \}$ defined in Appendix 7.4.

3.2. Main and adjoint problems

Based on adjoint variable method, the main problems of Problem 4 are introduced into the Reynolds Average Navier–Stokes Problem in Problem 3 and the eigenvalues problem of Snapshot POD in Problem 2. The adjoint problems of Problem 4 are given as follows.

Problem 5 (Adjoint Problem for $\omega$) After letting eigenfunction $\hat{u}$ of Problem 2 be given, then find $\alpha \in \mathbb{R}^{m \times m}$ such that

$$
\hat{u} \alpha = I,
$$  \hspace{1cm} (23)

and $\hat{u}, \alpha$ are the unitary matrix from Problem 5. Therefore, $\alpha$ is obtained as the inverse matrix or the transposed matrix of $\hat{u}$.

$$
\alpha = \hat{u}^{-1} = \hat{u}^T.
$$  \hspace{1cm} (24)

Problem 6 (Adjoint Problem for $\hat{u}$) Let the solution $u$ of Problem 1 be given with identify matrix $I$. Find $\alpha^T \in \mathbb{R}^{m \times m}$ such that

$$
\omega I \alpha^T = R(N_1, N_2, \hat{u}, \hat{u}) \alpha^T,
$$  \hspace{1cm} (25)
In fact, it is not necessary to solve Problem 6 because $\alpha$ has already been obtained in Problem 5.

**Problem 7 (Adjoint Problem for $$(\hat{\mathbf{u}}, \hat{\mathbf{p}})$$)** Let $\phi$ and the time-averaged solution $$(\hat{\mathbf{u}}, \hat{\mathbf{p}})$$ of Problem 1 and the eigenvalue and the eigenfunction $$(\omega, \hat{\mathbf{u}})$$ of Problem 2 be given. Find $$(\mathbf{w}, \mathbf{q}) : \Omega \rightarrow \mathbb{R}^d \times \mathbb{R}$$ such that

\[
\begin{align*}
(\nabla \mathbf{w}^T) \mathbf{w} - (\mathbf{u} \cdot \nabla) \mathbf{w} + \nabla \mathbf{q} - \frac{1}{Re} \Delta \mathbf{w} + \hat{\mathbf{A}} &= 0 \text{ in } \Omega, \\
\nabla \cdot \mathbf{w} &= 0 \text{ in } \Omega, \\
\mathbf{w} &= 0 \text{ on } \partial \Omega,
\end{align*}
\]

where

\[
\hat{\mathbf{A}} = 2 \sum_{i=1}^{m} \delta_{j=1}^{N} \alpha \Phi_{\omega}^{T}, \quad \hat{\mathbf{u}} = \sum_{n=N_1}^{N_2} \mathbf{u}^n, \quad \Phi_{\omega} = \Phi_{\omega}^{T}.
\]

Derivation of $\hat{\mathbf{A}}$ is presented in Nakazawa (2018).

**Problem 8 (Adjoint Problem for $\Phi_{\omega}$)** Let $\phi$ and the time-averaged solution $(\hat{\mathbf{u}}, \hat{\mathbf{p}})$ of Problem 1 and the eigenvalue and the eigenfunction $(\omega, \hat{\mathbf{u}})$ of Problem 2 with $\hat{\mathbf{u}} = \alpha^T$ be given. Find $\Phi_{\omega} : \Omega \rightarrow \mathbb{R}^d$ such that the following holds.

\[
\frac{\pi}{2} (\nabla \mathbf{w}^T)^T \Phi_{\omega} + 2 \Phi_{\omega} = 0
\]

In fact, it is not necessary to solve Problem 8 because $\Phi_{\omega}$ has already been obtained in Problem 2.

### 3.3. Sensitivity of the shape optimization problem

Here, based on the adjoint variable method, we evaluate the sensitivity of the shape optimization problem as

\[
G = \{(\mathbf{w} \cdot \nabla) \mathbf{w} - \frac{\pi}{4} \Phi_{\omega} (\Phi_{\omega})^T : \nabla \mathbf{w}^T + \frac{1}{Re} \nabla \mathbf{u}^T : \nabla \mathbf{w}^T \}
\]

By substituting $G$ into Eq. (38) and Eq. (39), Eq. (40), the sensitivity for the boundary integration type and the Generalized J integration type are evaluated.

### 4. Numerical Schemes

The Taylor–Hood (P2-P1) element pair for the velocity and pressure is used to discretize all equations spatially. FreeFEM++ (Hecht, 2012) is used for all numerical calculations.

The stationary solution $(\mathbf{u}^*, \mathbf{p}^*)$ is obtained to solve the stationary Navier–Stokes problem using the Newton–Raphson method. The non-stationary solution $\{(\mathbf{u}^n, \mathbf{p}^n)\}_{n=1}^{N}$ is obtained to solve Problem 1 with UMFPACK solver presented in Davis (2004) for every time step from $n = 1$ to $N$. For the term of the material derivative, the characteristic curve method which Notsu and Tabata Notsu et al. (2015) proved its mathematical proof and numerical availability, is used. The solver for the characteristic curve method is distributed in FreeFem++ (Hecht, 2012). After obtaining the non-stationary solution $\{(\mathbf{u}^n, \mathbf{p}^n)\}_{n=1}^{N}$, the correlation coefficient matrix $\mathbf{R}$ is formed for snapshot POD. The eigenvalue problem for the matrix $\mathbf{R}$ is solved in Problem 2 using lapack solver.

Based on the theory of the optimization problem considered herein, the adjoint problem of Problem 7 is solved to obtain $(\mathbf{w}, \mathbf{q})$ with the UMFPACK solver by Davis (2004). After evaluating the sensitivity, for domain deformation, the $H^1$ gradient method is used with UMFPACK solver (Davis, 2004). Finally, adaptive mesh refinement (AMR) is adopted, where adaptive mesh solver is distributed in Freefem++ (Hecht, 2012).

### 5. Numerical Calculations and Discussion

In this section, some parameters for numerical calculations are chosen in 5.1. Numerical calculation results are discussed in 5.2. From this section, the boundary and the volume, the Generalized J integration types are written as BI-type and VI-type, GJI-type.
5.1. Spatial and temporal discretization, adaptive mesh refinement

For comparison with numerical calculations in Nakazawa (2018), the same numerical accuracy is taken over as described below. Velocity and pressure are discretized in the spatial direction by finite element method, where nodes and elements are \((N_{\text{nodes}}, N_{\text{elements}}) = (21945, 43290)\). For discretization in time, the time step size \(\Delta t = 0.001\) is used to take time integrations of Problem 1 at \(Re = 100\). Velocity vectors are sampled from \(T_1 = 3\) to \(T_2 = 6\) for Snapshot POD. Additional details related to numerical accuracy can be found in Appendix A of an earlier report (Nakazawa, 2018). For AMR, see Appendix 7.6.

5.2. Numerical results

In this subsection, the only case of \(\delta_{2\rightarrow 4}\) is regarded as comparing an optimal domain in sensitivities of three kinds for BI-type and VI-type, GJI-type, for suppressing the time periodic flow and the normal stress because \(\delta_{2\rightarrow 4}\) is able to extract the time fluctuation component from a time-dependent flow using Snapshot POD. In fact, in the domain of interest, the power spectral density from the first to the fourth primary components is over 99% in Nakazawa (2018). Therefore, this paper is interested in the only primary components up to the fourth.

At first, the shape optimization problems is solved to compare results without and with AMR in the case of the BI-type. Fig. 2(a) and (b) are optimal shapes without and with AMR, and it is seemed that the sharp-edged boundary shape appears in the latter case. Fig. 3 depicts the cost function for without and with AMR, and that AMR is able to decrease the cost function more. From the result of Fig. 3, the optimal meshes for VI-type and GJI-type with using AMR are shown in Fig. 2(c) and (d). Fig. 2(c) for BI-type shows a pointy-haired shape, but Fig. 2(d) for GJI-type shows a partially relaxed-hair shape. Convergence histories of the cost function in BI-type and VI-type, GJI-type are shown in Fig. 4, where the cost function by VI-type is minimized at 25 step where GJI-type is performed. By the way, the third them of integrand in GJI-type is added compared to BI-type and VI-type, GJI-type are shown in Fig. 4, where the cost function by VI-type is minimized at 25 step where GJI-type is performed. Amr is able to decrease the cost function more. From the result of Fig. 3, the optimal meshes for VI-type and GJI-type with using AMR are shown in Fig. 2(c) and (d). Fig. 2(c) for BI-type shows a pointy-haired shape, but Fig. 2(d) for GJI-type shows a partially relaxed-hair shape. Convergence histories of the cost function in BI-type and VI-type, GJI-type are shown in Fig. 4, where the cost function by VI-type is minimized at 25 step where GJI-type is performed. By the way, the third them of integrand in GJI-type is added compared to VI-type, and the sign is minus as follows. As a result, the cost function is maximized in GJI-type.

\[
- (\nabla_v^T G)^T : [\nabla \phi^T \nabla \zeta].
\]  

(32)

Additionly, Fig. 5 shows \(\omega^1\) for validity of this numerical simulations.

Next, we present eigenvalues \(\Sigma^i_{l=2} \omega\) in the initial and the optimal domains for BI-type and VI-type, GJI-type in Table 1, and discuss efficiencies to suppress the time periodic flow. In fact, the eigenvalues over the second primary component \(\Sigma^4_{l=2} \omega\) represent the \(L^2\) norm of the time average velocity and the time fluctuation velocity vectors obtained by decomposing the time periodic flow into primary components. As a result of numerical calculation, the cost function of all of sensitivities are similar each other.

Finally, this paper adopts the following variable to compare normal stress on the design boundaries.

\[
\sigma(\partial \Omega_M) = \| - p_{\delta_{2\rightarrow 4}} \mathbf{v} + \frac{1}{Re} \nabla \cdot \mathbf{u}_{\delta_{2\rightarrow 4}} \|_{L^2(\partial \Omega_M)}.
\]

(33)

Therein, \(p_{\delta_{2\rightarrow 4}}\) denotes a corresponding pressure field to \(\mathbf{u}_{\delta_{2\rightarrow 4}} = \Sigma^4_{l=2} \Phi_\omega\). As shown in Table 2, \(\sigma\) in the optimal domain by the GJI-type is smaller than that by BI-type and VI-type.

<table>
<thead>
<tr>
<th>(\omega)</th>
<th>(\omega^1)</th>
<th>(\sigma(\partial \Omega_M)) for BI-type</th>
<th>(\sigma(\partial \Omega_M)) for VI-type</th>
<th>(\sigma(\partial \Omega_M)) for GJI-type</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Sigma^4_{l=2} \omega)</td>
<td>0.0285624359</td>
<td>0.020502601</td>
<td>0.020328633</td>
<td>0.02058691</td>
</tr>
</tbody>
</table>

Table 1. Eigenvalues \(\Sigma^4_{l=2} \omega\) in the initial and the optimal domains for BI-type and VI-type, GJI-type.

<table>
<thead>
<tr>
<th>(\omega)</th>
<th>(\omega^1)</th>
<th>(\sigma(\partial \Omega_M)) for BI-type</th>
<th>(\sigma(\partial \Omega_M)) for VI-type</th>
<th>(\sigma(\partial \Omega_M)) for GJI-type</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Sigma^4_{l=2} \omega)</td>
<td>0.170187</td>
<td>0.0777623</td>
<td>0.0866198</td>
<td>0.0777623</td>
</tr>
</tbody>
</table>

Table 2. Normal stress \(\sigma\) in the optimal domains for BI-type and VI-type, GJI-type.
Fig. 2 Finite element meshes (a) for BI-type without AMR, (b) for BI-type with AMR, (c) for VI-type with AMR, (d) for GJI-type with AMR.

Fig. 3 For $\delta_{2.4}$, normalized cost function $f^k/f^0$ for reshaping step $k = 45$ at $Re = 100$ in BI-type without and with AMR.

Fig. 4 For $\delta_{2.4}$, cost function for reshaping step at $Re = 100$ in BI-type and VI-type, GJI-type with AMR.
6. Conclusions

As described herein, the author extends a shape optimization method based on the sensitivity evaluated by
the General J Integral type from the optimal design techniques formulated in Nakazawa (2018) for suppressing
moderate time periodic flow fields at a low Reynolds number considering Reynolds Average Navier–Stokes
problem and Snapshot Proper Orthogonal Decomposition (Snapshot POD).

Particularly, the sum of eigenvalues in Snapshot POD is defined as the cost function. The non-stationary
Navier–Stokes problem and the eigenvalue problem in Snapshot POD are used as main problems. The main
problems are transformed from strong forms to weak forms with trial functions based on a standard framework
of the finite element method (FEM). The functional is described using the Lagrange multiplier method with
FEM. Next, using adjoint variable method, its material derivative is derived to evaluate the sensitivities of
two kinds evaluated by the boundary and the Generalized J integration types. The initial domain is iteratively
reshaped until the cost function satisfies the terminal condition, where the $H^1$ gradient method is used for stable
domain deformation.

For a numerical demonstration, a two-dimensional cavity flow is used with a disk-shaped isolated body.
Numerical results reveal that the optimal domain obtained using the Generalized J integration type is able to
decrease $\sigma$ more than that obtained using the boundary integration type, although both sensitivities decrease
the cost function similarly. In fact, the pointy-haired shape by the boundary integration type is obtained
because it does not meet mathematical regularity at the boundary. However, the Generalized J integration type
engenders a partially relaxed-hair shape because the mathematical regularity on the boundary is guaranteed.

7. Appendix

7.1. Material Derivative on Shape Optimization Problem

We examine a domain deformation $\phi$ as $\Omega \rightarrow \phi(\Omega)$, where $\phi$ is $\mathbb{R}^d$-valued function. For $|\varepsilon| \ll 1$, mapping $\phi$ is represented by $\phi = \phi_0 + \varepsilon \varphi$. Then we designate it by the identity map $\phi_0(\Omega) = \Omega$ and the domain variation $\varphi$. We assume $\zeta$ as a scalar-valued function describing a physical state in $\Omega$. For such $\zeta$, we introduce the following energy functional as

\[
L(\Omega, \zeta, \phi_0) = \int_\Omega G(x, \zeta) \, dx,
\]

where $G$ represents a real-valued given energy density function. The first variation of the functional for the
boundary integration type is

\[
\dot{L}(\bar{\Omega}, \zeta, \phi_0) = \int_\Omega G'(x, \zeta) \, dx + \int_{\partial \Omega} G \phi \cdot \nu \, d\Gamma,
\]

where $\cdot$ and $\cdot'$ respectively depict the material derivative and the Fréchet derivative with respect to $\zeta$, and
where $\nu$ represents the unit normal vector on the boundary. For the volume integration type,

\[
\dot{L}(\Omega, \zeta, \phi_0) = \int_\Omega G'(x, \zeta) \, dx + \int_\Omega \{ \varphi \cdot \nabla G + G(\nabla \cdot \varphi) \} \, dx.
\]

On the other hand, the following energy functional for the general J integration type is

\[
\dot{L}(\Omega, \zeta, \nabla \zeta, \phi_0) = \int_\Omega G'(x, \zeta) \, dx + \int_\Omega \{ \varphi \cdot \nabla G + G(\nabla \cdot \varphi) - (\nabla \cdot G)^\top : [\nabla \varphi^\top \nabla \zeta] \} \, dx.
\]
For sensitivity analysis, the adjoint variable method is used to derive a main problem and an adjoint problem by setting \( \oint G(\bm{x}, \zeta) \, dx = 0 \). After solving the main and the adjoint problems, density function \( G(\bm{x}, \zeta) \) is evaluated as sensitivity by substituting the main and adjoint variables into eq. (35) for the boundary integration type and eq. (36) for the volume integration type, eq. (37) for the general J integration type. As a result, we deduce the sensitivity for the boundary and the volume the Generalized J integration types, respectively as

\[
\dot{L}(\partial \Omega_m, \zeta, \phi) = \int_{\partial \Omega_m} G \phi \cdot \mathbf{v} \, dx,
\]

\[
\dot{L}(\Omega, \zeta, \phi) = \int_{\Omega} \{ \phi \cdot \nabla G + G(\nabla \cdot \phi) \} \, dx.
\]

\[
\dot{L}(\Omega, \zeta, \phi) = \int_{\Omega} \left\{ \phi \cdot \nabla G + G(\nabla \cdot \phi) - (\nabla_G G)^T : [\nabla \phi^T \nabla \zeta] \right\} \, dx.
\]

7.2. Constraint Function for Problem 1

Let \( (\mathbf{w}, q) \) be the adjoint variables with respect to the velocity and the pressure. By discretizing in the time direction with the finite difference method, a set of necessary variables is written as \( \zeta_1 = \{ \bm{u}, p, w, q \} \), where hereinafter \( \bm{u} = \{ u_j^{n_j} \}_{j=n_1}^{N_2}, \{ p_j^{n_j} \}_{j=n_1}^{N_2}, \{ \mathbf{q}_j^{n_j} \}_{j=n_1}^{N_2} \). The variational form of the non-stationary Navier–Stokes problem is defined as

\[
L_1(\Omega, \zeta_1) = - \sum_{n=n_1}^{N_2} \left\{ \int_{\Omega} G_1(x, \zeta_1) \, dx \right\}, \tag{41}
\]

by setting \( m = N_2 - N_1 + 1 \) with \( N_1 = \frac{T_1}{\Delta t} \) and \( N_2 = \frac{T_2}{\Delta t} \) for time step size \( \Delta t \), at time \( t = T_1, T_2 \). The density function \( G_1(x, \zeta_1) \) is presented as

\[
G_1(x, \zeta_1) = \frac{\mathbf{u}^{n+1}(x) - \mathbf{u}^n(x)}{\Delta t} \cdot \mathbf{w}^{n+1} - p^{n+1} \cdot \mathbf{w}^{n+1} - q^n \cdot \mathbf{u}^{n+1} + \frac{1}{Re} (\nabla \mathbf{u}^{n+1})^T : (\nabla \mathbf{w}^{n+1})^T, \tag{42}
\]

where \( \mathbf{X}^n = \mathbf{x} - \Delta t \mathbf{u}^n \), using the characteristic finite element scheme used in Notsu et al. (2015).

7.3. Constraint Function for Problem 2

For the optimization problem, let \( \zeta_2 = \{ \omega, \hat{u}, \alpha, \mathbf{u} \} \) be the set of necessary variables used in Problem 2, where \( \alpha \) is an adjoint variable for the eigenfunction \( \hat{\mathbf{u}} \).

\[
\alpha = [\alpha^1, \ldots, \alpha^i, \ldots, \alpha^m], \quad \alpha^i \in \mathbb{R}^m. \tag{43}
\]

The following functional is defined as

\[
L_2(\Omega, \zeta_2) = - \sum_{i=n_1}^{N_2} G_2(x, \zeta_2), \ G_2(x, \zeta_2) = \alpha \left[ \delta_{j \rightarrow k} \left\{ \omega I \hat{u} - \left( \int_{\Omega} \hat{u}^T \hat{u} \, dx \right) \hat{u} \right\} \right], \tag{44}
\]

where \( \delta_{j \rightarrow k} \) represents the weight function to extract \( j \) to the \( k \) primary components in 1 to the \( m \) primary components.

7.4. Constraint Function for Problem 3

Finally, we derive the following constraint function as the weak form based on the Reynolds Average Navier–Stokes Problem for \( \zeta_3 = \{ \hat{\mathbf{u}}, \hat{p}, \hat{\mathbf{w}}, \hat{q}, \Phi \mathbf{u} \} \),

\[
L_4(\Omega, \zeta_3) \simeq L_4(\Omega, \zeta_3) = - \int_{\Omega} \tilde{G}_1(x, \zeta_3) \, dx. \tag{45}
\]

Furthermore, the density function \( \tilde{G}_1(x, \zeta_3) \) is represented as

\[
\tilde{G}_1(x, \zeta_3) = (\hat{\mathbf{u}} \cdot \nabla \hat{\mathbf{u}}) \cdot \hat{\mathbf{w}} - \hat{C} : \nabla \hat{\mathbf{w}}^T - \hat{p} \mathbf{V} \cdot \hat{\mathbf{w}} - \hat{q} \mathbf{V} \cdot \hat{\mathbf{u}} + \frac{1}{Re} \nabla \hat{\mathbf{u}}^T : \nabla \hat{\mathbf{w}}^T, \tag{46}
\]

for the following expression

\[
\int_{\Omega} (\nabla \cdot \hat{C})^T \cdot \hat{\mathbf{w}} \, dx = - \int_{\Omega} \hat{C} : \nabla \hat{\mathbf{w}}^T \, dx, \tag{47}
\]

with \( \hat{\mathbf{w}} = 0_{\hat{p}, \hat{q}} \) on \( \partial \Omega \).
7.5. Derivation of the tensor for the time fluctuation term

This section describes deduction of the tensor for the time fluctuation term. The time fluctuation velocity \( \mathbf{u}_f(t) \) is represented as

\[
\mathbf{u}_f(t) = \sum_{i=2}^{m} \mathbf{\Phi}_\omega \mathbf{\tau}(t), \quad \mathbf{\Phi}_\omega = [\mathbf{\Phi}_\omega^1, \cdots, \mathbf{\Phi}_\omega^i, \cdots, \mathbf{\Phi}_\omega^m] \in \mathbb{R}^{d \times m}.
\]  

and \( \mathbf{\tau}(t) \) represents a time periodic function with a unity amplitude and with frequency to each POD mode \( i \).

Finally, we are able to derive tensor \( \mathbf{\tilde{C}} \) with \( \mathbf{\Phi}_\omega \) on a POD basis \( \mathbf{\Phi} \) and eigenvalue \( \omega \) as described below:

\[
\mathbf{\tilde{C}} = \int_{T_1}^{T_2} \mathbf{u}_f(t) \mathbf{u}_f(t)^T dt = \int_{T_1}^{T_2} \left\{ \sum_{i=2}^{m} \mathbf{\Phi}_\omega^i \mathbf{\tau}(t) \right\} \left\{ \sum_{i=2}^{m} \mathbf{\Phi}_\omega^i \mathbf{\tau}(t) \right\}^T dt
\]

\[
= \sum_{i=2}^{m} \left[ \int_{T_1}^{T_2} \left\{ \mathbf{\tau}(t) \right\}^2 dt \right] \mathbf{\Phi}_\omega^i \mathbf{\Phi}_\omega^i^T
\]

\[
= \pi \sum_{i=2}^{m} \mathbf{\Phi}_\omega^i \mathbf{\Phi}_\omega^i^T
\]

\[
= \frac{\pi}{4} \mathbf{\Phi}_\omega \mathbf{\Phi}_\omega^T,
\]

where one trigonometric identity engenders

\[
\int_0^{\frac{2\pi}{T}} \left\{ \mathbf{\tau}(t) \right\}^2 dt = \frac{\pi}{4}.
\]  

7.6. Adaptive Mesh Refinement

In this section, AMR distributed in Freefem++ (Hecht, 2012) is summarized as explained below.

A Taylor expansion of the data function \( \eta(x) \) with respect to any interior point \( x \) in an element over a mesh can be expressed as

\[
\eta(x) = \eta(x_c + i\delta x)
\]

\[
= \eta(x_c) + \{ (\nabla \eta)_{x=x_c} \}^T (i\delta x) + \frac{1}{2} (i\delta x)^T \{ (\nabla^2 \eta)_{x=x_c} \} (i\delta x) + o((\delta x)^3)
\]

\[
= \eta_h(x) + \frac{1}{2} (i\delta x)^T \{ (\nabla^2 \eta)_{x=x_c} \} (i\delta x) + o((\delta x)^3),
\]  

for \( t \in [0,1] \), where \( x_c \) represents the position vector at a node of an element in a mesh, and where \( \eta_h \) denotes the linear approximation for \( \eta \). The interpolation error \( e(x) \) at a displacement \( i\delta x \) from node \( x_c \) can be expressed as shown below.

\[
e(x) = \left| \int_0^t \left\{ \eta(x) - \eta_h(x) \right\} dt \right|
\]

\[
\approx \int_0^t \left| \frac{1}{2} (i\delta x)^T \{ (\nabla^2 \eta)_{x=x_c} \} (i\delta x) \right| dt
\]

\[
\leq \frac{1}{2} (\delta x)^T |(\nabla^2 \eta)_{x=x_c}| (\delta x) \int_0^t t^2 dt
\]

\[
= \frac{1}{6} (\delta x)^T |(\nabla^2 \eta)_{x=x_c}| (\delta x)
\]  

As described in this paper, after the domain is reshaped every reshaping step, an isotopic meshing is regarded as maintaining the same numerical accuracy as the initial domain over the mesh throughout this optimization process. Therefore, the Hessian matrix \( \nabla^2 \eta \) is the identity matrix for the case in which \( \eta = \frac{1}{2}(\delta x)^T(\delta x) \) is used. Finally, the maximal interpolation error over a mesh is written as

\[
e(x) = \frac{1}{6} h_{\text{max}}^2.
\]
where \( h_{\text{max}} \) represents the maximal length along all edges. The author works with only one variable denoted \( \eta \) for meeting the fixed error tolerance \( \varepsilon_h \) that must be equidistributed over the mesh

\[
\sup_{x \in \Phi(\Omega)} |\eta(x) - \eta_h(x)| \leq \frac{1}{6} \varepsilon_h. 
\]

(53)

The procedure of AMR distributed in Freefem++ is the following for \( i = 1 \cdots N_{\text{nodes}} \), where \( N_{\text{nodes}} \in \mathbb{N} \) denotes the number of nodes.

Step 1: Set \( i = 1 \) and \( \varepsilon_h \) arbitrarily.

Step 2: Let \( d_i \) be the length of edge \( a_i \).

Step 3: Compare \( \varepsilon_h \) and \( d_i \):
- If \( d_i > \varepsilon_h \) and \( i \leq N_{\text{nodes}} \), then the edge \( a_i \) must be cut into two edges; return to Step 2.
- If \( d_i \leq \varepsilon_h \) and \( i \leq N_{\text{nodes}} \), then replace \( i \) with \( i + 1 \); return to Step 2.
- Otherwise stop.

As described in this paper, \( \eta = \frac{1}{2} x^T x \) is used to evaluate the maximum interpolation error \( e(x) \) in triangles over mesh for longest edge length \( h_{\text{max}} \) in the initial mesh.

7.7. POD Basis

The following figures are stream functions of POD basis \( \Phi^i \) at the \( i \) primary components from \( i = 1 \) to \( 4 \).

![Stream functions of POD basis at \( i \)-th primary components from \( i = 1 \) to \( 4 \) at \( \text{Re} = 100 \) in the initial domain \( \Omega \).](image-url)

Fig. 6 Stream functions of POD basis at \( i \)-th primary components from \( i = 1 \) to \( i = 4 \) at \( \text{Re} = 100 \) in the initial domain \( \Omega \).
Fig. 7 For $\delta_{2\rightarrow i}$, stream functions of POD basis at $i$-th primary components from $i = 1$ to $i = 4$ at \( \text{Re} = 100 \) in the optimal domain $\phi(\Omega)$ with AMR and the boundary integration type.

Fig. 8 For $\delta_{2\rightarrow i}$, stream functions of POD basis at $i$-th primary components from $i = 1$ to $i = 4$ at \( \text{Re} = 100 \) in the optimal domain $\phi(\Omega)$ with AMR and the volume integration type.
For \(\delta_{i-4}\), stream functions of POD basis at \(i\)-th primary components from \(i = 1\) to \(i = 4\) at \(Re = 100\) in the optimal domain \(\phi(\Omega)\) with AMR and the Generalized J integration type.

References


